Chapter 2: Satellite instruments

Satellite remote sensors are instruments designed to obtain information on the atmospheric composition through the analysis of data acquired without direct contact with the atmosphere. While remote sensors can also be employed from the ground, balloon or aircraft, on satellites they provide a unique global view with a more comprehensive geographical coverage and regular observations. Satellite instruments can offer total column or height-resolved measurements. For this purpose, satellite instruments take advantage of different interactions of radiation with the atmosphere (*e.g.*, absorption, emission or scattering) and detect wavelengths throughout the electromagnetic spectrum. Disadvantages of satellite instruments are that they are often expensive, can be high risk, require complex space-qualified instrumentation, and have limited lifetimes.

In this chapter, *Section 2.1* presents a general discussion of the satellite measurement techniques and orbit types relevant for the instruments participating in the SPARC Data Initiative. More detailed descriptions of the specific instruments, including information on retrieval processes, are given in *Section 2.2*.

2.1 Satellite measurement techniques

The satellite instruments participating in the SPARC Data Initiative are all passive sensors. Passive sensors detect natural radiation emitted from an external source (*i.e.,* the sun or stars) or by the atmosphere itself. Active sensors, on the other hand, emit high-energy radiation themselves and detect what is reflected back from the atmosphere (*e.g.*, LIDARs). In this section, general characteristics of various passive remote sensing techniques are described in terms of measurement geometry and wavelength coverage, however the scope is limited to concepts relevant to this study.

Table 2.1 provides a classification of the instruments participating in the SPARC Data Initiative according to both categories (observation geometry and wavelengths), which are explained in more detail in *Sections 2.1.1* and *2.1.2,* respectively.

2.1.1 Classification by observation geometry

Satellite instruments can be classified according to their observation geometry into limb-viewing or nadir-viewing sounders. Limb sounders look tangentially through the atmosphere, while nadir sounders have a downward-viewing observation geometry, pointing towards the Earth's surface. Limb geometries are the natural choice for stratospheric measurements because the signal is not masked by the denser tropospheric signal, the long ray-path through the atmosphere provides large sensitivity to species with low atmospheric concentrations, and the variation of the observation angle allows vertical scanning of the atmosphere. As a result, altitude information on the observed atmospheric state variables can be obtained at high vertical resolution, while the horizontal resolution is limited. For tropospheric observations, limb measurements are more challenging because of the saturation of measured radiances and the opaqueness of the troposphere due to the presence of clouds, humidity, and generally larger density. For many aspects of tropospheric sounding, nadir sounders are advantageous, due to their small horizontal footprint.

In the following, limb-viewing sounders are further classified according to their measurement modes, which are based on emission, scattering, solar occultation, and stellar occultation. In parts of the satellite observation community the term 'limb sounding' is reserved for limb emission and limb scattering measurements, but here the term is used in a more general sense, including the occultation geometry. A description of the nadir emission technique is also provided.

Limb emission

Emission measurements in limb geometry record the signal that is emitted along a horizontal path through the atmosphere and is partly absorbed on its way between the emitting air parcel and the observer (see **Figure 2.1**). Variation of the elevation angle of the line-of-sight (LOS) allows altitude-resolved temperature and composition measurements from approximately cloud-top height to the thermosphere. In turn, the horizontal resolution is limited to ~300 km unless corrections for LOS gradients are applied, or tomography is used. Since the Planck function at terrestrial temperatures is very low for wavelengths shorter than about 2.5 μm, limb emission measurements are, at least under conditions of local thermodynamic equilibrium, feasible only at wavelengths larger than this threshold, *i.e.,* in the mid-infrared to the microwave spectral region. At these wavelengths, atmospheric scattering is negligible except for clouds and large aerosol particles. Since, in contrast to occultation measurements (see

Table 2.1: Instruments classified according to observation geometry and wavelength categories. *Only instruments participating in the SPARC Data Initiative, and the measurement modes considered, are listed.*

	Microwave / Sub-mm 100 µm - 10 cm	Mid-IR 2.5 - 20 µm	Near-IR 0.8 - 2.5 µm	VIS / UV < 0.8 µm
Limb emission	UARS-MLS Aura-MLS SMR SMILES	MIPAS HIRDLS LIMS		
Solar occultation		ACE-FTS HALOE	POAM II/III SAGE I/II/III	POAM II/III SAGE I/II/III ACE-MAESTRO
Stellar occultation				GOMOS
Limb scattering			SCIAMACHY	SCIAMACHY OSIRIS
Nadir emission		TES		

below), no direct illumination source is needed, emission measurements can be obtained during both day and night. Depending on the orbit of the platform, measurements can be performed globally with dense spatial coverage, and the azimuth angle can be arbitrarily chosen as long as the Sun is avoided. A disadvantage of the emission technique compared to occultation measurements is the relatively small signal to noise ratio, which is caused by the faint signal of atmospheric emission. Calibration and determination of the exact elevation angle of the LOSs are crucial to avoid propagation of related errors onto the retrieved trace gas abundance profiles. Within the SPARC Data Initiative, the limb emission technique is used by Aura-MLS, HIRDLS, LIMS, MIPAS, SMILES, SMR, and UARS-MLS.

Solar occultation

Solar occultation instruments record radiance emitted by the Sun and attenuated along a horizontal ray-path through the atmosphere by extinction, *i.e.,* absorption and scattering (see **Figure 2.2**). Similar to the limb emission measurements, altitude-resolved information is obtained by variation of the elevation angle of the LOS. However, in contrast to limb emission where the measurement geometry can be freely chosen, the geometry is defined by the position of the Sun with respect to that of the satellite and the Earth. Measurements in occultation geometry can only be performed during the sunrise and sunset as seen from the satellite, *i.e.,* two times per orbit, which results in a limited global coverage and greatly reduced data density (compared to an emission sounder). On the other hand, the Sun provides a large radiance signal, allowing highly precise measurements even at shorter wavelengths. Occultation measurements are usually performed at wavelengths from the UV to the mid-IR. These measurements are self-calibrating in a sense that the division of atmospheric spectra by direct Sun (*e.g.*, exo-atmospheric) spectra yields transmission spectra. Within the SPARC Data Initiative, solar occultation is represented by ACE-FTS, ACE-MAESTRO, HALOE, POAM II/III, and SAGE I/II/III.

Stellar occultation

Stellar occultation measurements use the same concept as solar occultation measurements, except that stars act as the radiation source instead of the Sun (see **Figure 2.2**). Since multiple stars can be used, this results in a larger data density compared to that achieved by solar occultation. Night-time measurements are of better quality than daytime measurements because the scattered solar signal interferes with the target signal of the stars during daytime. The useful spectral range is limited to wavelengths below about 1 µm. At longer wavelengths terrestrial thermal emission interferes with the stellar signal. Weak stellar radiation and scintillations from atmospheric irregularities are particular challenges of stellar occultation techniques. Within the SPARC Data Initiative, stellar occultation is represented by GOMOS.

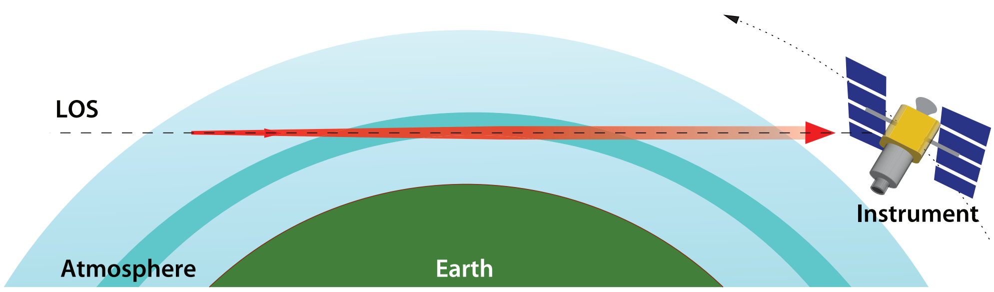

Figure 2.1: Limb emission observation geometry. *The instrument measures radiation emitted by the atmosphere along the LOS.*

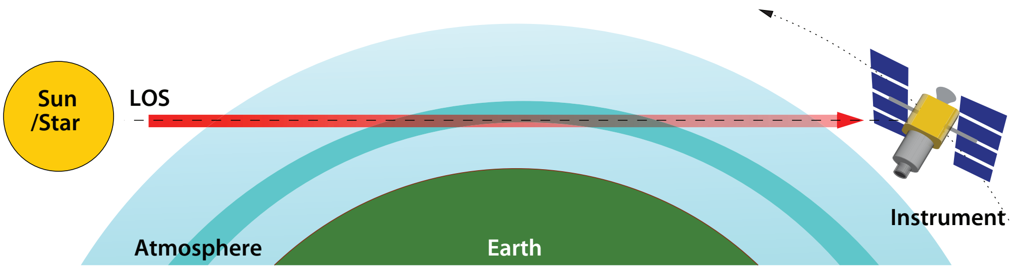

Figure 2.2: Occultation observation geometry. *The instrument points at the radiation source (the Sun or a star) and measures the radiation attenuated along the LOS.*

Limb scattering

The radiance received by limb scattering instruments consists of photons originating from the Sun and scattered into the field-of-view of the instrument (see **Figure 2.3**). The information on the atmospheric state is provided by the scattering itself, or by the absorption of scattered photons along their way through the atmosphere. In contrast to the measurement techniques discussed above, the ray-path is not defined by the measurement geometry, but is scattered by the atmosphere into the LOS of the instrument. As for all measurement techniques using the Sun as the source of the signal, measurements are only possible during daylight. On the sunlit part of the globe, good spatial coverage is achieved. The vertical resolution is similar to that of limb emission and solar occulation instruments. Measurements are made in the UV to the near-infrared range where scattering is relevant. Within the SPARC Data Initiative, limb scattering is represented by OSIRIS and SCIAMACHY.

Nadir emission

Nadir observations are measurements for which the LOS points down to the surface of the Earth. The signal received by nadir emission instruments can contain photons emitted by the Earth's surface or atmosphere and transmitted through the atmosphere. In contrast to limb measurements, for which vertically resolved measurements are achieved simply by variation of the elevation angle of the LOS, the altitude information of nadir observations is given by pressure broadening of spectral lines and by varying opacity at different wavelengths. While the altitude resolution is far inferior to that of limb sounders, the horizontal resolution is better, and allows more measurements between clouds that can penetrate lower into the troposphere. The LOS through the atmosphere is shorter than in limb sounding, which reduces sensitivity to low abundance species but also reduces opacity problems. Infrared nadir sounding is possible during both day and night, but thermal contrast has an impact on altitude resolution and sensitivity to the abundance of species in the lower troposphere. Nadir infrared measurements require on-board blackbody calibration and a space view for cold space calibration measurements. Uncertainties in surface emissivity can complicate the retrieval process. Within the SPARC Data Initiative, nadir emission measurements are represented by TES. Note that TES is the only nadir-viewing instrument considered by the SPARC Data Initiative. TES evaluations presented in this report account for the relatively broad averaging kernel of the instrument and serve as an example for the more comprehensive comparisons that would be needed when considering nadir instruments (such instruments include, for example SBUV, TOMS, and MOPITT).

2.1.2 Classification by wavelengths

The different instruments can, in addition to the classification by observation geometry, be classified according to the spectral range in which they operate. Wavelengths used for atmospheric composition measurements range from the microwave to the ultraviolet spectral region. Instruments contributing to the SPARC Data Initiative include both radiometers, which measure a signal spectrally integrated over certain frequency bands, and spectrometers, which provide spectrally resolved measurements. Better spectral resolution allows measurement of trace gas species with weaker spectral signatures. On the other hand, the advantage of lower spectral resolution is a higher signal-to-noise ratio for single measurements, which helps to provide better spatial resolution.

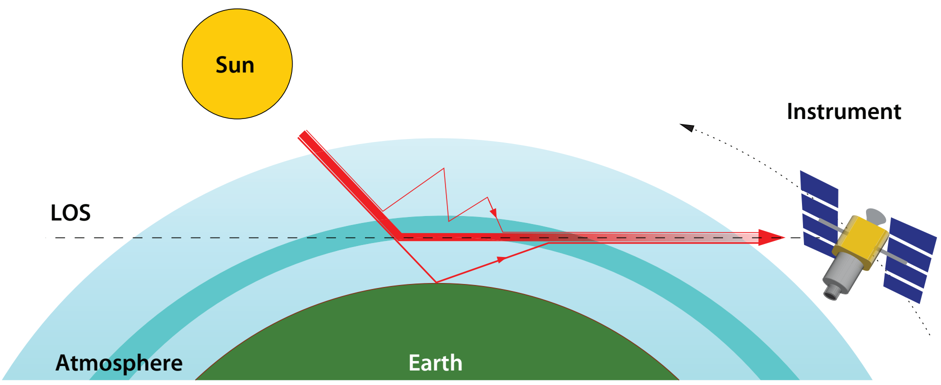

Figure 2.3: Limb scattering observation geometry. *The instrument measures radiation emitted by the Sun and scattered into the field-of-view.*

Table 2.2: Atmospheric constituents and the wavelength bands they are detected by the instruments used in this study.

Species / Wave-length bands	O_3	H_2O	CH_4, CCl_3F, CCl_2F_2, HF, SF_6, HNO_4, N_2O_5, $ClONO_2$, $BrONO_2$, CH_2O	N_2O, CO, NO, HNO_3, HCl, ClO, HOCl	NO_2	HO_2, CH_3CN	BrO	Aerosol
Microwave/ Sub-mm	X	X		X		X	X	
Mid-IR	X	X	X	X	X			
Near-IR		X						X
VIS / UV	X				X		X	X

Table 2.2 lists the atmospheric constituents together with the wavelength bands in which they are observed by the instruments participating in the SPARC Data Initiative. In the following, the main characteristics of the different wavelength bands are briefly described.

Microwave and sub-millimeter

The microwave and sub-millimeter spectral region covers wavelengths from 10 cm to 100 µm. This corresponds to frequencies of about 3 GHz to 3 THz, respectively. The sources of radiation are rotational transitions of molecules with a permanent dipole moment. The temperature dependence of microwave and far-infrared emissions is lower than in the mid-infrared, and clouds are not as much of an interference in the former than in the latter. Measurements are not sensitive to aerosol particles or thin clouds. The typical measurement mode is emission sounding. Within the SPARC Data Initiative this spectral region is represented by Aura-MLS, SMILES, SMR, and UARS-MLS.

Mid-infrared

The mid-infrared spectral region covers wavelengths from about 2.5-20 µm, corresponding to wavenumbers from about 4000-500 cm^{-1}. The sources of the signal are rotational-vibrational transitions of molecules with a transitional dipole moment. The temperature dependence of these transitions is high and the frequency range covers the maximum of the Planck function at terrestrial temperatures. Clouds are less transparent in the mid-infrared than in the microwave spectral region. Radiative transfer is dominated by emission and absorption, while scattering is only an issue in the presence of clouds or elevated aerosol levels. Emission sounding is possible and often applied at wavelengths longer than about 4 µm (non-local thermodynamic equilibrium emission can also be detected at shorter wavelengths), but solar absorption measurements are common as well. Within the SPARC Data Initiative, this spectral region is represented by ACE-FTS, HALOE, HIRDLS, LIMS, MIPAS, and TES.

Near-infrared, visible and ultraviolet

In the near-infrared spectral region (wavelengths 0.8-2.5 µm, wavenumbers 12500-4000 cm^{-1}), overtone and combined vibrational transitions give rise to the signal, while in the visible (0.4-0.8 µm) and ultraviolet (below 0.4 µm) spectral regions, emission is caused by electronic transitions. The maximum of the Planck function of the effective temperature of the Sun's photosphere is in the visible spectral range, while emission at terrestrial temperatures at these wavelengths is negligible. Thus, remote sensing in this spectral region relies on absorption and scattering of signal emitted by hot background sources like the Sun or stars. Within the SPARC Data Initiative, this spectral region is represented by ACE-MAESTRO, GOMOS, OSIRIS, POAM II/III, SAGE I/II/III, and SCIAMACHY.

2.1.3 Satellite orbits

Stratospheric composition sounding is currently performed exclusively from low Earth orbit (LEO), platforms flying at altitudes between approximately 300 and 2000 km above the Earth's surface. The latitude coverage of the orbit is determined by its inclination, *i.e.,* the angle between the orbit plane and the equatorial plane. Polar orbits (*e.g.*, that of Envisat) with inclinations near 90° provide global coverage and allow observation of the polar regions. Many of these satellites are in sun-synchronous orbits, *i.e.,* orbits where measurements at a given geo-location on either the ascending or descending segments of the orbit have approximately the same local solar time (LST). Therefore, sun-synchronous satellites cannot provide information on the diurnal variation of the state of atmosphere at any fixed latitude. Instruments within the SPARC Data Initiative that were/are flying on sun-synchronous satellites are Aura-MLS, GOMOS, HIRDLS, LIMS, MIPAS, OSIRIS, POAM II/III, SAGE III, SCIAMACHY, SMR, and TES. Non-sun-synchronous orbits allow Earth observation at different local times but lead to temporally varying datasets. This can be an issue when creating climatologies, particularly for species with pronounced diurnal variations. Instruments within the SPARC Data Initiative that were/are flying on non-sun-synchronous satellites/platforms are ACE-FTS, ACE-MAESTRO, HALOE, SAGE I/II, SMILES, and UARS-MLS.

2.2 Instrument and retrieval descriptions

The satellite instruments participating in the SPARC Data Initiative are all passive sensors using a limb viewing observation geometry with the exception of one nadir-viewing sounder used for particular upper troposphere/lower stratosphere (UTLS) studies (see *Section 4.27*). The measurement modes of the limb-viewing sounders (emission, scattering, solar occultation, and stellar occultation) determine data coverage and sampling density.

Retrieval processes include a so-called forward model and an inversion algorithm. The forward model computes radiances that would be observed given a state vector of atmospheric composition and temperature profiles. The inversion algorithm then "inverts" these calculations and solves for an atmospheric state from a given set of radiance observations. In many cases (ACE-FTS, Aura-MLS, HALOE, HIRDLS, LIMS, MIPAS, SMR, TES, UARS-MLS), initial retrievals of temperature and pressure are performed using observations of molecules whose abundances are well known (usually CO_2 in the infrared and O_2 in the microwave). Temperature and pressure can be retrieved as separate products if the emission lines are strong enough (*e.g.*, SMILES, SMR). Some instruments (*e.g.*, OSIRIS, SAGE II, SCIAMACHY) rely on meteorological analyses for temperature profile information. In either case, accurate knowledge of tangent altitude/pressure is required for limb measurements.

Uncertainties are typically provided by the operational retrieval systems, but they generally do not include systematic effects such as the propagation of spectroscopic uncertainties. Beyond such uncertainties, retrieval constraints (*e.g.*, smoothing) affect the altitude resolution and lead to an imperfect representation of the true atmospheric state. Available validation information is provided separately for each molecule in *Chapter 4*.

In the following, the different instruments together with their retrieval processes are described, in order of their launch date, with the earliest instrument first.

2.2.1 LIMS on Nimbus 7

Nimbus 7 was launched on October 24, 1978, and carried a number of instruments for making measurements of the state of the middle atmosphere. The Limb Infrared Monitor of the Stratosphere (LIMS) experiment was a limb-infrared sounder, focused on measurements of temperature, O_3, and those species that affect ozone (H_2O, NO_2 and HNO_3) [see *Gille and Russell*, 1984]. Nimbus 7 was in a sun-synchronous orbit with a noon and midnight equator crossing time. However, LIMS was designed to look off-plane, so that the measurements were made near 1pm and 11pm local time at equator crossing. The resulting sampling pattern can be found in Figure 10 of *Gille and Russell* [1984]. The temperature and ozone profiles extend from cloud-top to near the mesopause, while the profiles of H_2O, HNO_3, and NO_2 are restricted to the stratosphere, due to their signal-to-noise (S/N) limitations. The cryogen gases that were used to cool the detectors only lasted until May 28, 1979, as planned. Thus, the LIMS dataset extends for about 7.5 months and consists of daily, orbital profiles from about 64°S to 84°N latitude. The data were processed with a Version 5 algorithm and archived in 1982 at NASA Goddard. More recently, the algorithm was revised to Version 6, and new retrievals were conducted and archived at the Mirador site of the Goddard Earth Sciences and Data Information Services Center (GES DISC) or at **http://daac.gsfc.nasa.gov** and can be downloaded *via* ftp from there. A separate LIMS website exists at **http://www.gats-inc.com/projects.html#lims** for viewing daily plots of the data. Descriptions of the quality of the Version 6 temperature, O_3, H_2O, and HNO_3 and NO_2 can be found in *Remsberg et al.* [2004, 2007, 2009, and 2010], respectively.

Retrievals for the LIMS V6 temperature *versus* pressure (or $T(p)$) profiles are described in *Remsberg et al.* [2004] and references therein. The algorithm uses a top-down, onion-peeling approach and iterates to achieve a match of the calculated and measured radiances for its wide and narrow CO_2 radiometer channels in the 15-μm region. A constant CO_2 mixing ratio profile was assumed for the forward radiance models. Radiance profiles for the LIMS species channels are registered with pressure according to the associated $T(p)$ profiles, and their forward models account for the retrieved temperatures. Level 2 profiles of the temperature and species volume mixing ratio (VMR) are tabulated at 18 levels per decade of pressure or at a spacing of 0.88 km. They have an effective vertical resolution of 3.7 km. The retrieval algorithm for NO_2 accounts for interfering radiances from H_2O, CH_4, and the oxygen continuum in the 6-7 μm region. The algorithm for HNO_3 accounts for interfering radiances from the primary CFC molecules and from aerosol emissions in the 11-μm region.

2.2.2 SAGE I on AEM-B, SAGE II on ERBS, and SAGE III on Meteor-3M

The Stratospheric Aerosol and Gas Experiment (SAGE) series of instruments consists of four instruments including the Stratospheric Aerosol Measurement (SAM II) that span the period from 1978 through 2005. All of the instruments use solar occultation to measure attenuated solar radiation through the Earth's limb during satellite sunrise and sunset. The first instrument in the series, SAM II on-board Nimbus 7 (1978-1993), consisted of a single 1000-nm aerosol channel with measurements restricted to high latitudes (>53° in both hemispheres). Note, SAM II is not included in the evaluations of this report. SAGE I on-board AEM-B (1979-1981) consisted of four measurement channels (corresponding to wavelengths of 385, 450, 600, and 1000 nm), which were used to infer aerosol extinction profiles at two wavelengths (450 and 1000 nm) and O_3 and NO_2 concentration profiles. SAGE II on-board ERBS (1984-2005) made measurements at seven wavelengths (385, 448, 452, 525, 600, 940, and 1020 nm) from which O_3, NO_2, H_2O and aerosol extinction at four wavelengths (385, 452, 525, and 1020 nm) were retrieved [*McCormick et al.*, 1989]. SAGE III on-board the Russian Meteor-3M satellite was launched on December 2001 and remained operational into December 2005. It used an 800 element Charged Coupled Device (CCD) linear array detector to provide continuous spectral coverage between 280 and 1040 nm. An additional single photodiode at 1550 nm was used for aerosol extinction measurements. The SAGE III measurements at 87 channels between 285 and 1545 nm were used to infer vertical profiles of O_3, NO_2, H_2O, and aerosol extinction at nine wavelengths (285, 448, 521, 602, 676, 755, 868, 1019, and 1545 nm) [*Thomason and Taha*, 2003].

Both SAGE I and II instruments were in inclined (~57°) orbits that permitted near-global coverage over the course of 30 to 40 days (see **Figure 2.4**). There are 15 sunrise and 15 sunset measurements each day that cover a narrow latitude band and are separated by ~24° in longitude. Unlike SAGE I and II, where sunrise and sunset measurements alternatively observe the Northern and Southern Hemispheres, all SAGE III sunrise measurements occur in the Southern Hemisphere (30°S to 60°S) while all sunset

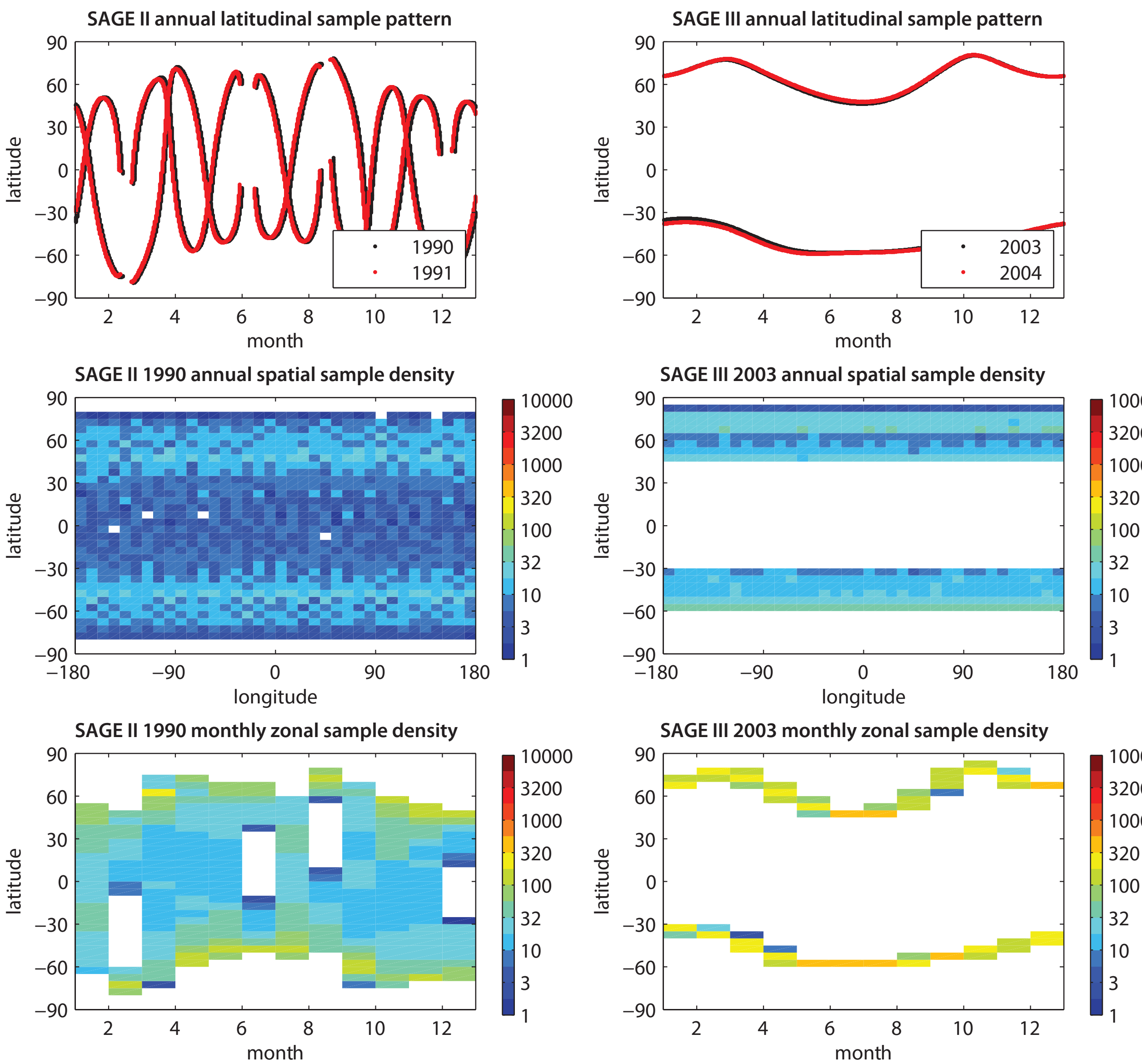

Figure 2.4: Sampling pattern and resulting sample density for SAGE II (left) and SAGE III (right). *Note, SAGE I provided similar geographical and temporal sampling as SAGE II. For SAGE III, sunrise measurements occur in the Southern Hemisphere, and sunset events occur in the Northern Hemisphere.*

measurements occur in the Northern Hemisphere (40°N to 80°N) due to its sun-synchronous orbit (see **Figure 2.4**).

SAGE III additionally operated in lunar occultation mode from which O_3, NO_2, NO_3, and OClO were derived. Currently no aerosol product is produced from lunar occultation measurements. Since there are fewer lunar occultation data from SAGE-III, only measurements from solar occultation are used to create the climatologies used in this report.

An aerosol climatology was developed by the SPARC Assessment of Stratospheric Aerosol Properties (ASAP) and is available on the SPARC Data Centre website (**http://www.sparc-climate.org/data-centre/**). Months during 2005 that are missing on this website are available by request from Larry Thomason (l.w.thomason@nasa.gov).

The retrieval of trace gas profiles from SAGE measurements is accomplished by taking the following major steps. First the solar radiance at all measured wavelengths along with spacecraft ephemeris data are processed to produce slant path optical depth profiles as a function of tangent height. The total slant path optical depth at a particular wavelength is a linear combination of Rayleigh scattering and other contributed trace gases (*e.g.*, O_3, NO_2, and aerosol). The contribution of Rayleigh scattering is first removed from the total slant path optical depth before an inversion algorithm is applied to optimally account for the contribution of other measured gases. Detailed descriptions of retrieval algorithms for SAGE I, SAGE II, and SAGE III can be found in *Chu and McCormick* [1979], *Chu et al.* [1989] and SAGE III ATBD [2002], respectively. The native data files can be found *via* the NASA LaRC data website **http://eosweb.larc.nasa.gov/**.

2.2.3 HALOE on UARS

The Halogen Occultation Experiment (HALOE) was launched on-board the Upper Atmosphere Research Satellite (UARS) on September 12, 1991. The HALOE instrument performed flawlessly over the UARS lifetime through November 2005. The UARS was in a 600-km near-circular orbit with a 57° inclination. HALOE used the solar occultation technique and the instrumental methods of gas-filter radiometry to measure vertical profiles of HF (2.45 μm), HCl (3.4 μm), CH_4 (3.46 μm) and NO (5.26 μm), and broadband radiometry to measure vertical profiles of NO_2 (6.25 μm), H_2O (6.6 μm), O_3 (9.6 μm), and temperature *versus* pressure with approximately 2.3 km vertical resolution. HALOE also measured aerosol extinction in the four gas-filter channels. The altitude coverage is species-dependent, but is limited to within the 10-150 km range. HALOE measured 15 sunrise and 15 sunset events per day and achieved near-global coverage in approximately a month. The daily measurement spacing was equal in longitude and varied seasonally in latitude. The HALOE measurement sampling was influenced over the lifetime of the mission by: 1) drifts in the UARS orbit; 2) the power-sharing mode among UARS instruments due to a malfunction of the solar array in May 1995; 3) reduced battery power in June 1997; and 4) difficulties with the spacecraft tape-recorder mechanism in October 1999. For a detailed description of the HALOE measurement and retrieval techniques, see *Russell et al.* [1993]. The sampling pattern and resulting measurement density from HALOE can be seen in **Figure 2.5**.

The HALOE temperature retrieval assumes a CO_2 concentration that varies based on the annual CO_2 increase rate determined form ground-based and *in situ* measurements. The observed 3570 cm^{-1} transmission is matched in an upward, hydrostatically-constrained process. This is iterated several times, with intervening profile registrations. Above ~85 km, temperatures from the MSIS model [*Hedin*, 1991] are assumed, and below ~35 km NCEP temperatures are used. The 1510, 1600 and 1015 cm^{-1} radiometer channels are used to retrieve NO_2, H_2O, and O_3, respectively, in an

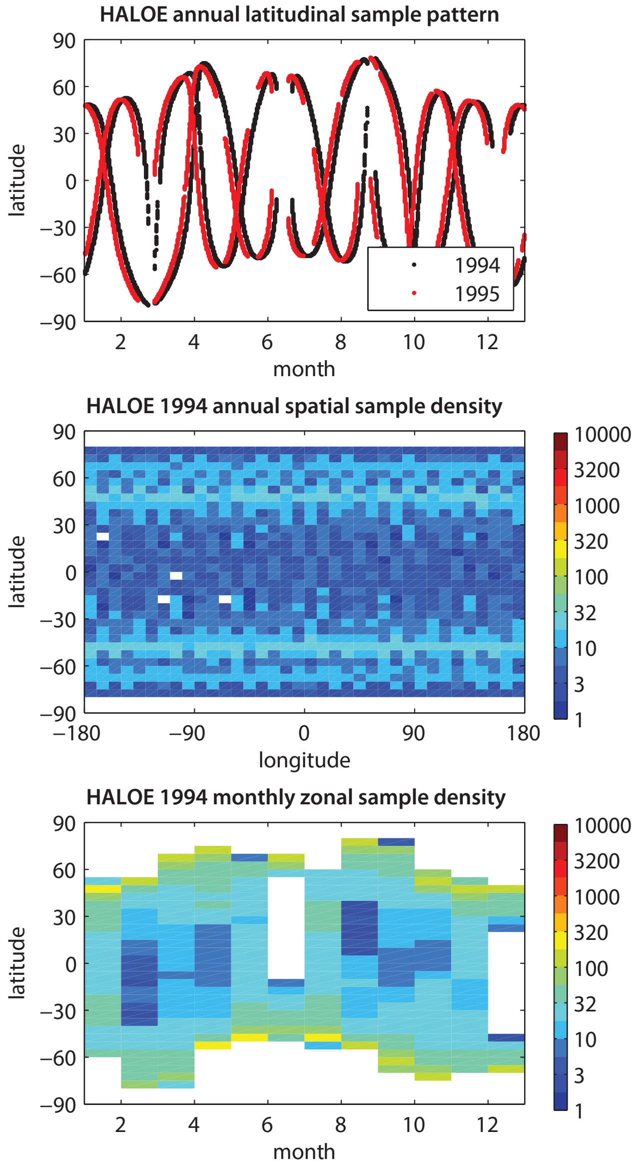

***Figure 2.5:** Sampling pattern and resulting sample density for HALOE.* *Note that the sampling pattern shifts from year to year.*

onion-peeling fashion. The Gas Filter Radiometer differential technique is used to retrieve HF, HCl, CH_4, and NO from the 4080, 2940, 2890, and 1900 cm^{-1} channels. In these channels, the light is split. Half is sent through a cell filled with the target gas, and the other half through a vacuum path. The exo-atmospheric difference of these signals is balanced to within the noise levels. The difference-signal that develops when viewing through the atmosphere is highly sensitive to atmospheric absorption from the target gas, but virtually insensitive to aerosol absorption. The aerosol extinction is retrieved from the 1900 cm^{-1} (*i.e.,* NO channel) vacuum-path signal and extrapolated to the radiometer channels assuming a sulphate model to account for the sensitivity to aerosols at these wavelengths. The spectroscopy used in the HALOE forward model is based on HITRAN 1991–1992. The HALOE algorithm has gone through two major revisions. The initial HALOE validation results for each species were published in 1996 [*Russell et al.*, 1996a, 1996b; *Gordley et al.*, 1996; *Harries et al.*, 1996; *Hervig et al.*, 1996a, 1996b; *Park et al.*, 1996; *Brühl et al.*, 1996]. The HALOE processing version used in the SPARC Data Initiative is the third public release (V19) which can be obtained from the following website: **http://haloe.gats-inc.com/home/index.php**. Numerous satellite science teams have used HALOE V19 to compare and validate their instruments [*e.g.*, *Randall et al.*, 2003; *Froidevaux et al.*, 2006] and this version has been extensively used in previous SPARC reports [*e.g.*, *SPARC*, 2000]. In addition, a comprehensive stratospheric climatology of O_3, H_2O, NO_x, HF, HCl, and CH_4 was developed from HALOE V19 measurements by *Grooß and Russell* [2005].

2.2.4 MLS on UARS

UARS-MLS was one of ten instruments on the UARS platform, launched on 12 September 1991 as mentioned in *Section 2.2.3* [*Reber et al.*, 1993]. UARS-MLS (a predecessor to Aura-MLS) pioneered microwave limb sounding of the Earth's stratosphere and mesosphere from space. It was designed to measure stratospheric O_3, H_2O and ClO, but also provided stratospheric and mesospheric temperature, and stratospheric HNO_3 (as well as upper tropospheric humidity and other information not used in this report). UARS-MLS measured millimeter-wavelength thermal emission as the antenna was vertically scanned (every 65.54 s) from about 1 to 90 km through the atmospheric limb [*Barath et al.*, 1993; *Waters et al.*, 1993]. There were typically 26 limb views during each 65-s scan. The vertical resolution as constrained by the field-of-view is ~3 km, and the UARS-MLS data (for the data versions used here) are produced on a vertical grid with a resolution of ~2.7 km. The spatial resolution is about 400 km along the LOS, and about 7 km across. UARS-MLS used three radiometers to measure the microwave emission near 63, 205, and 183 GHz. The radiances in each band were measured by one of six identical spectrometer filter-banks, each consisting of 15 contiguous channels, covering up to ±255 MHz away from the line centre. The channels vary in width from 2 MHz near the line centre to 128 MHz in the wings.

The UARS orbit was inclined at 57° and the satellite performed a 180° yaw maneuver 10 times per year, at approximately 36 day intervals. The UARS-MLS measurements cover 34° on one side of the equator to 80° on the other side, with hemispheric coverage switching with each yaw maneuver. The orbit precession ensured that the measurements covered essentially all LSTs during each 36 day interval. Profiles were spaced ~3-4° along the orbit track and the average daily sampling in longitude was ~12°. Coverage was denser near the turn-around latitudes. The main operational events affecting the time series from UARS-MLS were the mid-April 1993 failure of the 183-GHz radiometer, resulting in the loss of stratospheric H_2O (and 183-GHz O_3 observations), and the mid-June 1997 cessation of 63-GHz observations in order to save spacecraft power, resulting in a loss of the temperature information. The frequency of MLS operational days generally decreased over the mission, from close to 100% from late 1991 through 1993, down to about 50% in late 1994, and only several tens of

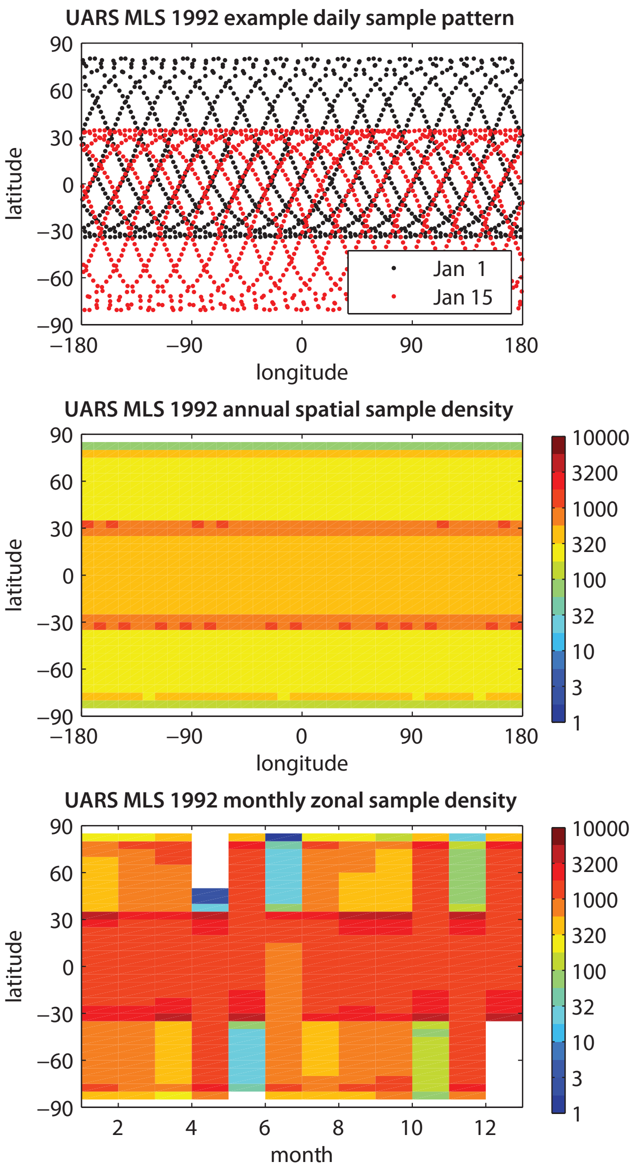

Figure 2.6: Sampling pattern and resulting sample density for UARS-MLS.

measurement days per year from 1995 onward; the last retrievals were obtained on 25 August 2001. The relevant (O_3, ClO, HNO_3) UARS-MLS data are therefore generally considered most robust for "long-term" series analyses until mid-June 1997; we have included data through 1999 for this report and the related database. The sampling pattern and resulting measurement density from UARS-MLS can be seen in **Figure 2.6**, for one of the early years (with best coverage).

The UARS-MLS retrieval algorithms are based on the optimal estimation approach [*Rodgers*, 1976, 2000]. These algorithms make use of two different forward models; one is a complete line-by-line radiative transfer model, and the other is based on a Taylor series computation using precomputed output from the full model. The standard UARS-MLS products are temperature, H_2O, O_3, HNO_3, ClO, and CH_3CN. The Version 5 data were the last major public release of UARS MLS data, however, updates and improvements were made available for H_2O and HNO_3 [see *Livesey et al.*, 2003], which is why we have used a Version 6 file label for these two species. For stratospheric H_2O, the work of *Pumphrey* [1999] and *Pumphrey et al.* [2000] demonstrated the value of using the originally-named V0104 dataset (also used here and referred to as V6), rather than V5 H_2O. UARS-MLS stratospheric H_2O mixing ratios are typically flagged as bad for pressures larger than 100 hPa. Moreover, there are no valid data after the month of April, 1993, as the radiometer measuring stratospheric H_2O failed that month.

The original data files used to produce the climatological files are the standard Level 3AT UARS MLS daily files. These files contain data on a subset of the standard "UARS" pressure surfaces, which are evenly spaced with six surfaces per decade change in pressure (or about 2.7 km), although the true resolution is typically somewhat coarser. In addition, Level 3TP "Parameter files" are produced for each day of MLS observations. These files contain information on the quality of the UARS-MLS data. The supplementary material from *Livesey et al.* [2003] gives more information on the implementation of the UARS-MLS retrieval algorithms, as well as data screening guidelines; the mixing ratio profiles (*versus* pressure) were screened accordingly, interpolated vertically, and averaged to obtain the monthly zonal means used here. The general guidelines for the proper use of UARS-MLS data (see *Livesey et al.* [2003]) have been followed, namely: 1) only data whose associated uncertainty is positive should be used; 2) only profiles where the MMAF_STAT diagnostic field is set to G, T, or t should be used; 3) only profiles where the appropriate QUALITY field is equal to 4 should be used; and 4) the spike information given on the MLS science team website should also be used for removing outliers. The official public distribution location for UARS-MLS data used here is (as for Aura-MLS) at the NASA GES-DISC Mirador website, namely **http://mirador.gsfc.nasa.gov**. Public information about both MLS instruments, data access, and MLS-related publications, can be found at the MLS website (**http://mls.jpl.nasa.gov**).

2.2.5 POAM II on SPOT-3 and POAM III on SPOT-4

The Polar Ozone and Aerosol Measurement II (POAM II) instrument was launched on-board the French SPOT-3 satellite on 26 September 1993 into a 98.7° inclination, sun-synchronous orbit at an altitude of 833 km. The instrument operated between October 1993 and November 1996 when the SPOT-3 satellite suffered a malfunction and contact with the instrument was terminated. POAM III was launched on the French SPOT-4 spacecraft on 24 March 1998 into an orbit identical to the one of SPOT-3. The instrument began taking data on 22 April 1998 and operated until 5 December 2005, when instrument failure terminated the mission. POAM III was functionally very similar to its predecessor, although it contained a number of design changes that improved sensitivity and accuracy. POAM II and III both used the solar occultation technique, measuring the extinction of solar radiation in nine narrow-band channels from approximately 350 to 1060 nm and 353 to 1018 nm, respectively, to retrieve the vertical distribution of atmospheric O_3, H_2O, NO_2, and aerosol extinction. Over their mission lifetimes, POAM II and III compiled datasets of approximately 21,000 and more than 43,000 good occultation profiles, respectively. POAM II and III made 14 measurements per day in each hemisphere, equally spaced in longitude around a circle of approximately constant latitude. Satellite sunrise measurements were made in the Northern Hemisphere and sunsets in the Southern Hemisphere. Sunrise measurements occur in a latitude band from 55-71°N while sunsets occur between 63-88°S. The latitude coverage changes slowly with season and is exactly periodic from year to year. The sampling patterns of POAM II and III are shown in **Figure 2.7**.

Vertical resolution of the POAM data products is approximately 1 to 1.5 km, depending on the species. The altitude range also varies by species and instrument version; for POAM II O_3 (15-50 km), NO_2 (20-40 km) and aerosols (10-30 km), and for POAM III O_3 (5-60 km), NO_2 (20-40 km), H_2O (5-45 km) and aerosols (5-25 km). Note that unlike POAM II, POAM III also provided a water vapour product that was thoroughly validated against a variety of correlative satellite-, aircraft- and balloon-borne datasets. Due to uncertainties in the optical filters for the differential water vapour channels, water vapour was never retrieved operationally from POAM II measurements.

A complete discussion of the POAM II instrument can be found in *Glaccum et al.* [1996]. The Version 6 algorithms, error analysis and data characterisation are described by *Lumpe et al.* [1997]. A discussion of the POAM III instrument can be found in *Lucke et al.* [1999]. The Version 4 algorithms, error analysis and data characterisation are described by *Lumpe et al.* [2002]. The final public release datasets for POAM II (V6.0) and POAM III (V4) are available at the NASA Langley Atmospheric Sciences Data Center (**http://www.eosweb.larc.nasa.gov**) and are also distributed by the Naval Research Laboratory *via* **https://www.nrl.navy.mil/rsd/7220/poam-ftp**.

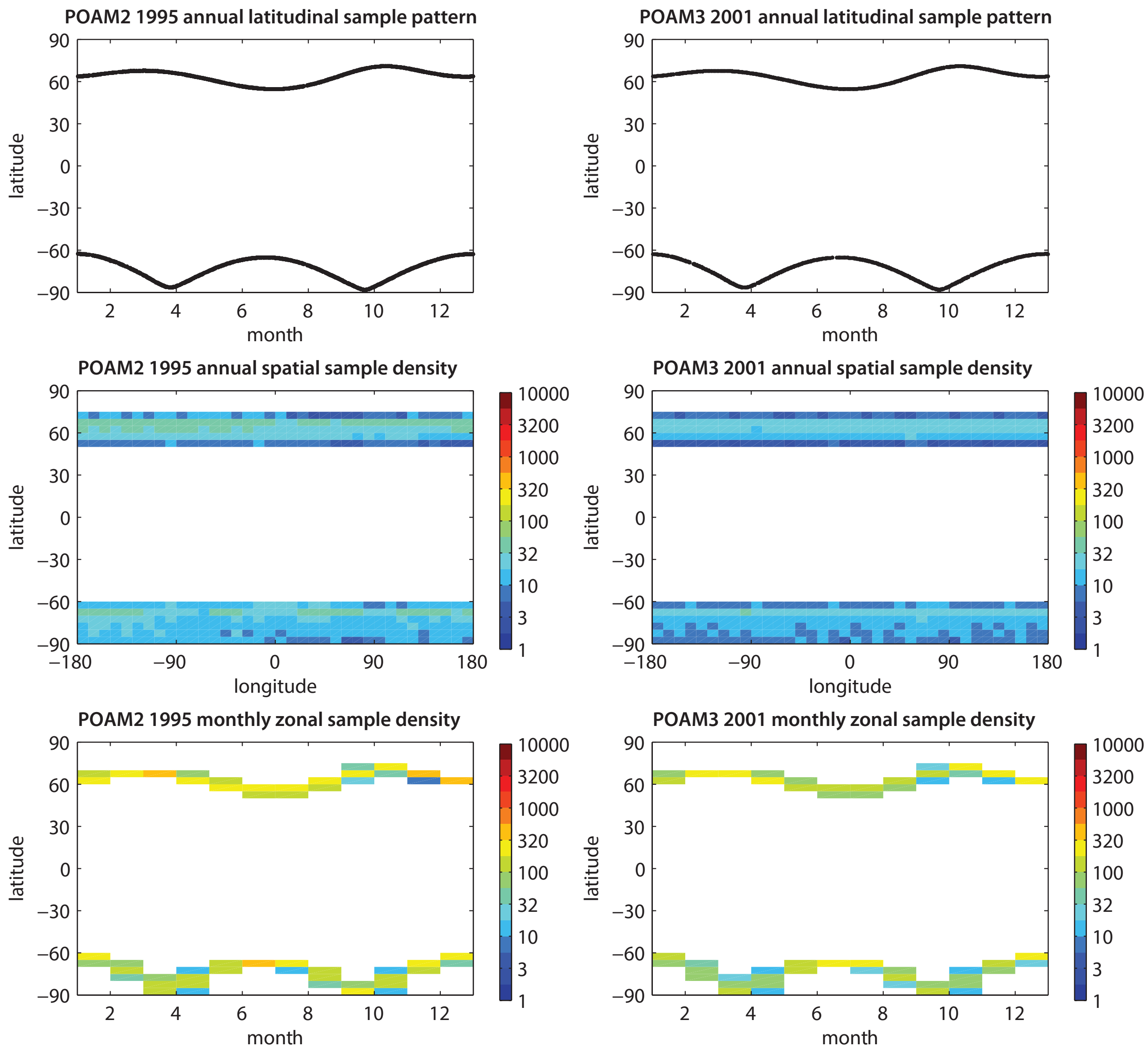

Figure 2.7: Sampling pattern and resulting sample density for POAM II (left) and III (right).

POAM measures limb profiles of slant-path transmission in nine spectral channels from roughly 350 to 1000 nm. Using this input data stream the algorithms retrieve vertical profiles of O_3, NO_2, H_2O, and O_2 (or total) density, as well as aerosol extinction between 350 and 1000 nm (POAM II did not retrieve H_2O or total density – see above). All atmospheric species are retrieved simultaneously using an optimal estimation algorithm (fixed, non-varying *a priori* for all species; constraints are tuned to minimise retrieval variability at the desired vertical resolution). The conversion of transmission data to geophysical profiles is achieved *via* a two-step process, beginning with a spectral inversion to partition the various gas and aerosol components of the measured total slant optical depth, followed by a spatial inversion to produce altitude profiles of gas density and aerosol extinction from the path integrated quantities. The NO_2 and H_2O retrievals use closely spaced differential absorption pair channels in the UV and Near-IR, respectively, while O_3 is retrieved from a single channel at the peak of the Chappuis band at 602 nm. Aerosols are retrieved at all wavelengths by constraining the spectral dependence to a quadratic in log-log space (optical depth *versus* wavelength).

Both instruments included an O_2 A-band channel designed to provide self-consistent temperature/pressure retrievals, however they were never made operational (the POAM II channel saturated, while POAM III had an unresolved systematic bias presumably due to bandpass characterisation errors). The POAM III retrievals used the Rayleigh scattering signal in the 350-nm channel to retrieve total density above 30 km and hence remove the background Rayleigh scattering self-consistently from all channels. Below 30 km the density is tightly constrained to the United Kingdom Meteorological Office (UKMO) analysis. The POAM II retrievals were constrained to fix the total density to the UKMO analysis (co-located in time and space) due to an unresolved overall altitude grid error.

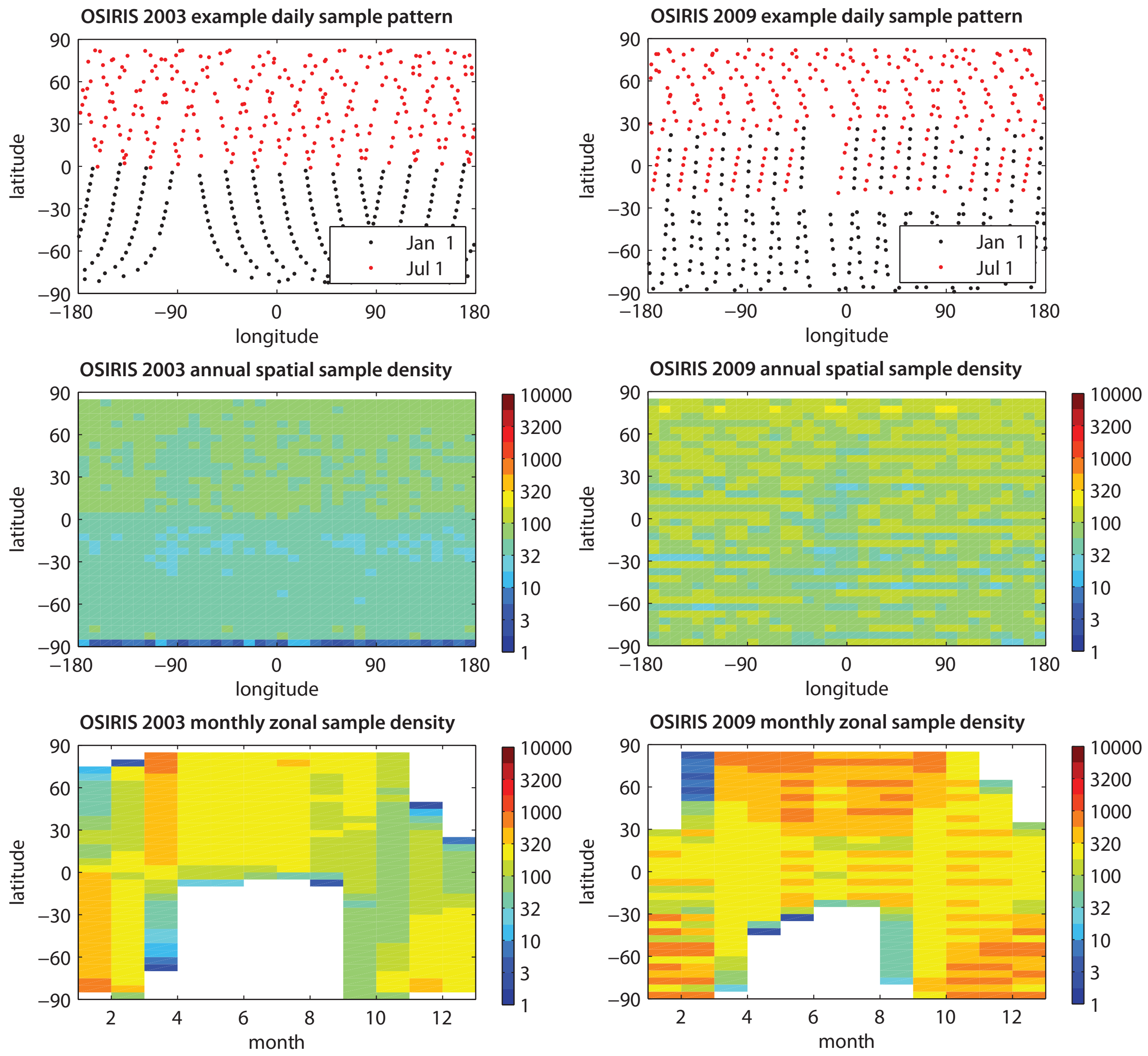

***Figure 2.8:** Sampling pattern and resulting sample density for Odin/OSIRIS for 2003 and 2009.*

2.2.6 OSIRIS on Odin

The Odin satellite was launched on 20 February 2001 into a 600-km circular sun-synchronous near-terminator orbit with a 97.8° inclination [*Murtagh et al.*, 2002]. Odin carries two instruments: the Optical Spectrograph and InfraRed Imager System (OSIRIS) [*Llewellyn et al.*, 2004] and the Sub-Millimetre Radiometer (SMR; see *Section 2.2.7*) [*Frisk et al.*, 2003]. The instruments are co-aligned and scan the limb of the atmosphere through controlled nodding of the satellite over a tangent height range from 7 to 70 km in approximately 85 s (stratospheric mode, ~65 scans per orbit) or from 7-110 km in about 140 s (stratospheric-mesospheric mode, ~40 scans per orbit). Due to Odin's orbit, the data from both instruments are generally limited to between 82°N and 82°S except for occasional short periods of off-plane pointing at high latitudes during early polar spring. The LSTs of the observations are close to 6pm and 6am for low and mid-latitudes during the ascending and descending nodes respectively, but sweep quickly over local midnight and noon at the poles. Moreover, the equator crossing times are slowly drifting in LST during the Odin mission. A particularity of the Odin satellite is that observation times were initially equally shared between astronomical and atmospheric observation modes. The astronomy mission ended in April 2007 and since then Odin has been entirely dedicated to atmospheric sciences.

OSIRIS is a grating spectrometer that measures limb-scattered sunlight spectra in the spectral range from 280 nm to 800 nm at a resolution of about 1 nm. The scattered sunlight measurements are used to provide vertical profiles of minor stratospheric constituents including O_3, NO_2, BrO and aerosol. Additional datasets exist, but only the official products are mentioned here. Since OSIRIS observations are dependent on sunlight, the full latitude range is only covered around the equinoxes and hemispheric coverage is provided elsewhere. Examples of daily and annual sampling distributions are shown in **Figure 2.8.**

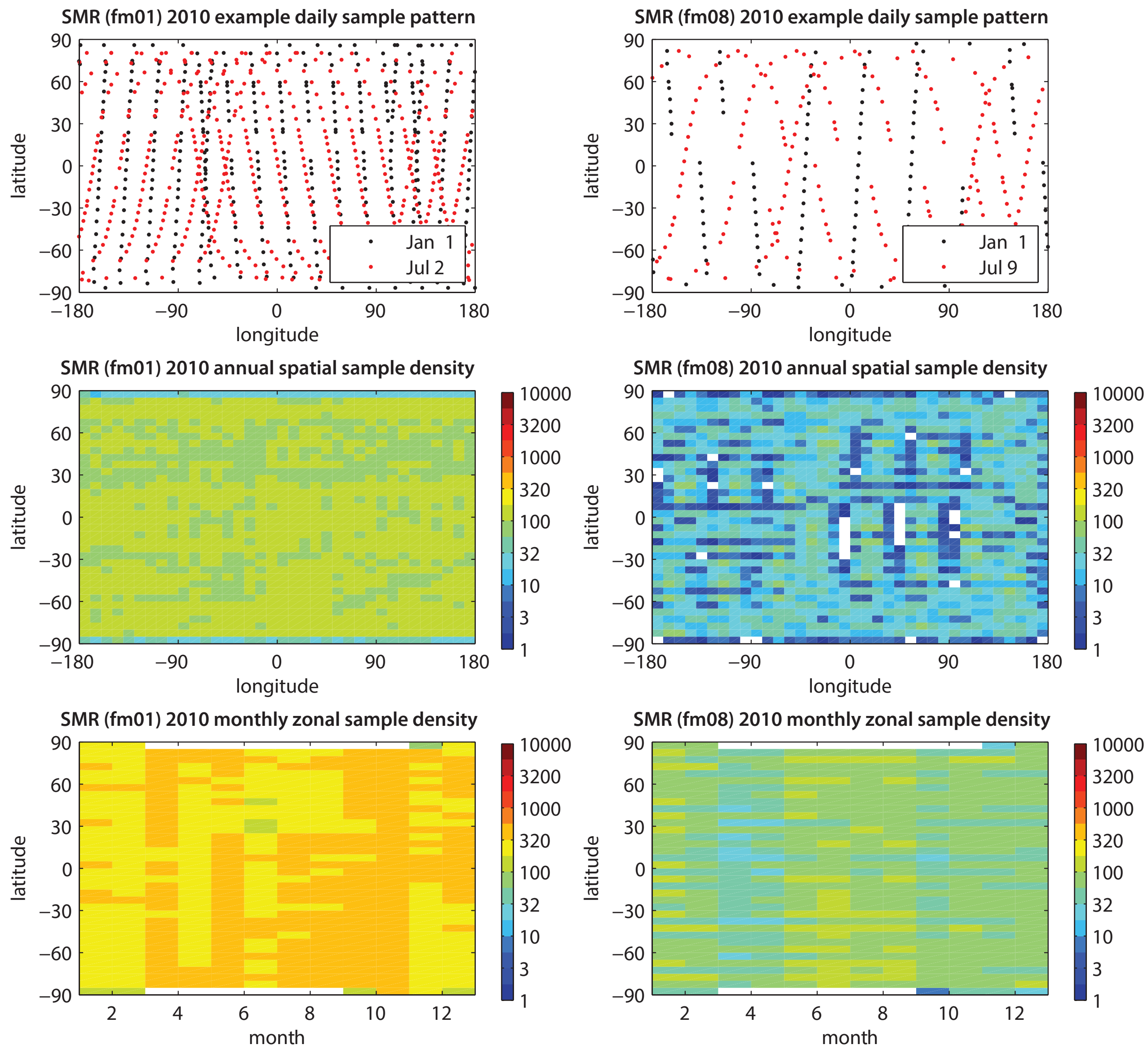

Figure 2.9: Typical sampling pattern and resulting sample density for Odin/SMR for 2010. *Left: stratospheric mode; Right: water isotope mode (H_2O-16). Note that the sampling density increased from April 2007 when the Odin astronomy mission ended.*

The NO_2 (V3.0) product is retrieved using a combination of DOAS and the log-space optimal estimation method using wavelengths between 435 and 451 nm [*Haley et al.*, 2004; *Brohede et al.*, 2007a; *Haley and Brohede* 2007]. BrO (V5) is also retrieved with optimal estimation, but on zonally-averaged OSIRIS spectra, in the 346-377 nm range [*McLinden et al.*, 2010]. Ozone (V5) is retrieved with a multiplicative algebraic reconstruction technique (MART) using a range of doublet/triplets in the Hartley and Huggins bands [*Degenstein et al.*, 2009]. OSIRIS ozone profile measurements show agreement with coincident SAGE II occultation measurements to within 2% from 18 to 53 km altitude over a large range of geo-locations and solar zenith angles. Stratospheric aerosol (V5) is also retrieved using a MART algorithm where the retrieval vector is designed to enhance the extra scattering, above the Rayleigh background, due to sulphate aerosols [*Bourassa et al.*, 2007]. For this vector a wavelength ratio of 750 nm to 470 nm is used to characterise the effect of the Mie scattering signal. Hydrated sulphuric acid particle microphysics, including a size distribution for typical background aerosol, are assumed to calculate the scattering cross section and phase functions that are required to retrieve the aerosol extinction. The altitude range and resolution vary for each species and profile but are usually limited to the stratosphere and a maximum of ~2 km vertical resolution.

Inferred NO_y, NO_x and Br_y data products are also compiled using OSIRIS data, combined with photochemical box-model simulations for each individual profile [*Brohede et al.*, 2008; *McLinden et al.*, 2010], although Br_y is not presented in this report. Note that HNO_3 observations from the Odin/SMR instrument are also used in the NO_y product (NO_2+NO+HNO_3+$ClONO_2$+2*N_2O_5). The NO_x dataset (NO_2+NO) is not explicitly described in the literature but is compiled using box-model scaling factors, following the approach in *Brohede et al.* [2008]. Previous climatology studies and model inter-comparisons with OSIRIS data are described by *Brohede et al.* [2007b] for NO_2, *McLinden et al.* [2010] for BrO/Br_y and *Brohede et al.* [2008] for NO_y. See the OSIRIS official website for more information and data access: **http://osirus.usask.ca/.**

2.2.7 SMR on Odin

The Sub-Millimetre Radiometer (SMR) on-board the Odin satellite (for launch and orbit details, see *Section 2.2.6*) uses four sub-millimetre and 1-millimetre wave radiometer to measure thermal emission from the atmospheric limb in the 486-581 GHz spectral range and around 119 GHz [*Murtagh et al.*, 2002; *Frisk et al.*, 2003]. The signal is collected by a 1.1 m telescope and spectrally analysed by two auto-correlator spectrometers, each with 800 MHz bandwidth and 2 MHz effective resolution. Stratospheric mode observations of O_3, ClO, N_2O, HNO_3, and H_2O in the UTLS are performed using two bands around 501 and 544 GHz on every third observation day (on every other day since April 2007) [*e.g.*, *Urban et al.*, 2005a, 2006; *Urban*, 2008; *Ekström et al.*, 2008]. Other regular observation modes are dedicated to the measurements of target species in the middle atmosphere such as water and ozone isotopologues around 490 GHz [*Urban et al.*, 2007; *Jones et al.*, 2009], mesospheric and lower thermospheric H_2O at 557 GHz [*Urban et al.*, 2007; *Lossow et al.*, 2009; *Orsolini et al.*, 2010], stratospheric and mesospheric CO, O_3 and HO_2 around 576 GHz [*Dupuy et al.*, 2004; *Jin et al.*, 2009; *Baron et al.*, 2009], and H_2O-17, O_3, and NO in a band at 551 GHz [*Urban et al.*, 2007]. For example, water isotope mode observations of H_2O^{16} were performed on 1 day per week until 2007 (10 days per month since April 2007). The sampling pattern and resulting measurement density from SMR for the stratospheric mode and the water isotope mode can be seen in **Figure 2.9**.

Vertical profiles (Level-2 data) are retrieved from the calibrated spectral measurements of the limb scans (Level-1b data) by inverting the radiative transfer equation for a non-scattering atmosphere. Employed retrieval techniques for Odin/SMR Level-2 processing are based on the optimal estimation method (except for upper tropospheric humidity and ice) [*Urban et al.*, 2004; *Buehler et al.*, 2005; *Eriksson et al.*, 2005]. The altitude range and resolution varies for each species depending on the signal-to-noise ratio and frequency band employed. Currently recommended data versions are V2.0 for the 544 GHz band and V2.1 for all other modes.

Climatologies of several species (N_2O, HNO_3, NO_2, NO_y, CO, ClO, O_3), derived from Odin observations since 2001 and compiled in terms of altitude or equivalent latitude *versus* pressure, altitude, or potential temperature, are available from the Odin/SMR website (**http://odin.rss.chalmers.se**). For information on the climatologies of HNO_3, NO_2, and derived NO_y the reader is referred to *Urban et al.* [2009], *Brohede et al.* [2007a] and *Brohede et al.* [2008].

2.2.8 GOMOS on Envisat

GOMOS (Global Ozone Monitoring by Occultation of Stars) was a stellar occultation instrument on-board the European Space Agency's Environmental satellite, Envisat [*Bertaux et al.*, 2010; **http://envisat.esa.int/handbooks/gomos/**]. Envisat was launched into its sun-synchronous polar orbit of 98.55° inclination at about 800 km altitude on 1 March 2002. Contact to the satellite was lost on 8 April 2012. Its equator crossing time was 10am. For every occultation GOMOS first measured a star's reference spectrum when the star was seen above the atmosphere. This reference spectrum and the spectra measured through the atmosphere were used to calculate the horizontal transmission spectra through the atmosphere. Transmissions are the basis for spectral and vertical retrieval of species profiles. GOMOS performed 100-200 night occultations per day. The measurement coverage of night occultations was global, except in the

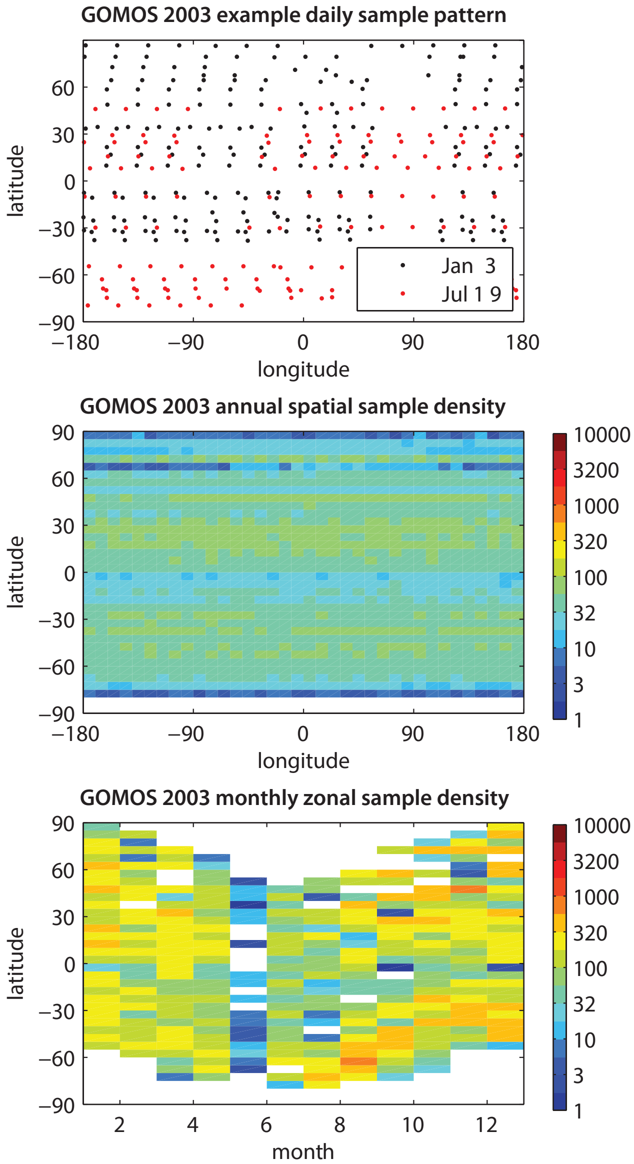

Figure 2.10: Sampling pattern and resulting sample density for GOMOS.

summer-time polar regions. Daytime occultations were also measured, but they are not used in the present work due their lower quality. Measurements start at 150 km and extend down to 5 km in cloudless conditions. The altitude-sampling resolution is 0.5-1.7 km and depends on the azimuth of the LOS with respect to the orbital plane. The nominal vertical resolution of the retrieved ozone profiles is 2 km below 30 km, 2-3 km between 30-40 km and 3 km above 40 km, and for other species about 4 km (see also *Section 3.1.3.8*). The instrument optical design was based on a 30-cm telescope that simultaneously fed UV-VIS and IR spectrometers, two fast photometers and two redundant star trackers. Spectra were recorded by CCD detectors. The UV-VIS spectrometer spectral range were 250-690 nm with 0.3 nm sampling and 0.9 nm resolution. The constituents retrieved are O_3, NO_2, NO_3, and aerosol. The IR spectrometer channels are 750-776 nm and 916-956 nm with 0.06 nm sampling and 0.1 nm resolution. IR data are used to retrieve O_2 and H_2O. Two fast (1 kHz) photometers at blue and red wavelengths were used to make the scintillation correction for the spectrometer data, retrieve high-resolution temperature profile and probe stratospheric turbulence.

The self-calibrating measurement principle with good vertical resolution and accurate vertical geo-location made GOMOS a good candidate to produce long time series and climatologies (see *Hauchecorne et al.* [2005], *Kyrölä et al.* [2006, 2010a, 2010b], *Vanhellemont* [2010]). However, difficulties with the pointing system in 2003, 2005 and 2009 have left some gaps in the data coverage. Noise levels of the CCDs increased steadily from the launch date, and this has led to a decrease in the quality of data over time. The sampling pattern and resulting measurement density from GOMOS can be seen in **Figure 2.10**.

The climatologies are constructed using GOMOS data from ESA processing Version IPF 5. The retrieval scheme is discussed in *Kyrölä et al.* [2010b]. The GOMOS constituent profile retrieval starts from the horizontal transmission spectra. Occultations are processed one at a time. The data processing is split into Level 1b and Level 2 stages. In Level 1b, dark charge removal and other instrumental corrections are performed and finally transmission spectra are constructed. Geo-location is determined starting from the satellite location and from the known direction of the star, and performing ray-tracing calculations with the atmosphere assumed to be the one given by the ECMWF data below 1 hPa and the MSIS90 climatology in the upper atmosphere. In Level 2 processing, the transmission spectra are first corrected for dilution caused by refraction and for modulations by scintillations. The fast photometer data are used in the scintillation correction. In case of off-orbital-plane occultations, the correction is not able to remove the scintillation modulation arising from isotropic turbulence in the LOS. The ozone retrieval, however, is only weakly sensitive to modulations by scintillations [*Sofieva et al.*, 2010]. Ozone as well as NO_2, NO_3, and aerosols are retrieved from the UV/VIS range 250-675 nm. The Rayleigh extinction is removed using the ECMWF+MSIS90 data. The UV/VIS retrieval is divided into two consecutive stages. In the spectral inversion the model transmission function is fitted by a non-linear Levenberg-Marquardt method to the transmissions. Because of perturbations caused by uncorrected isotropic scintillations, NO_2 and NO_3 retrievals are based on sub-iteration using the differential cross section method [see *Hauchecorne et al.*, 2005].

After spectral inversion the vertical inversion is performed using so-called onion-peeling method. The inversion is constrained using the target resolution Tikhonov method [*Sofieva et al.*, 2004]. For ozone the target vertical resolution is 2 km below 30 km and 3 km above 40 km. For other constituents the target vertical resolution is 4 km. An iteration loop over spectral and vertical inversion is performed in order to take into account the temperature dependence of the cross sections. The retrieval errors for constituent profiles depend on the brightness of the star measured. For ozone, the error depends also on the spectral type of the star. Data quality and error estimates of GOMOS are discussed in detail in *Tamminen et al.* [2010].

2.2.9 MIPAS on Envisat

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) was a mid-infrared Fourier transform limb emission spectrometer designed and operated for measurement of atmospheric trace species from space [*Fischer et al.*, 2008]. It was part of the instrumentation of Envisat (for launch and orbit details, see *Section 2.2.8*). MIPAS passed the equator in a southerly direction at 10am local time 14.3 times a day, observing the atmosphere during day and night with global coverage from pole to pole. The instrument's field of view was 30 km in the horizontal and approximately 3 km in the vertical direction. MIPAS covered the 4.3-15 μm region in five spectral bands: band A (685-970 cm^{-1}), AB (1020-1170 cm^{-1}), B (1215-1500 cm^{-1}), C (1570-1750 cm^{-1}), and D (1820-2410 cm^{-1}).

MIPAS operated during July 2002 – March 2004 at full spectral resolution of 0.035 cm^{-1} (unapodised) in terms of full width at half maximum. During this period, MIPAS recorded a rear-viewing limb sequence of 17 spectra each 90 seconds, corresponding to an along track sampling of approximately 500 km and providing about 1000 vertical profiles per day in its standard observation mode. Tangent heights covered then the altitude range from 68 down to 6 km with tangent altitudes at 68, 60, 52, 47, and then at 3 km steps from 42 to 6 km.

Due to problems with the interferometer-mirror-slide system, MIPAS performed few operations from April–December 2004. In January 2005 regular observations resumed, but with a reduced duty cycle and a reduced spectral resolution of 0.0625 cm^{-1}. These new measurements have the advantage that more spectra could be measured during the same time interval compared to the former "high"-spectral resolution observations. Tangent heights covered the range from 70 down to 6 km with tangent

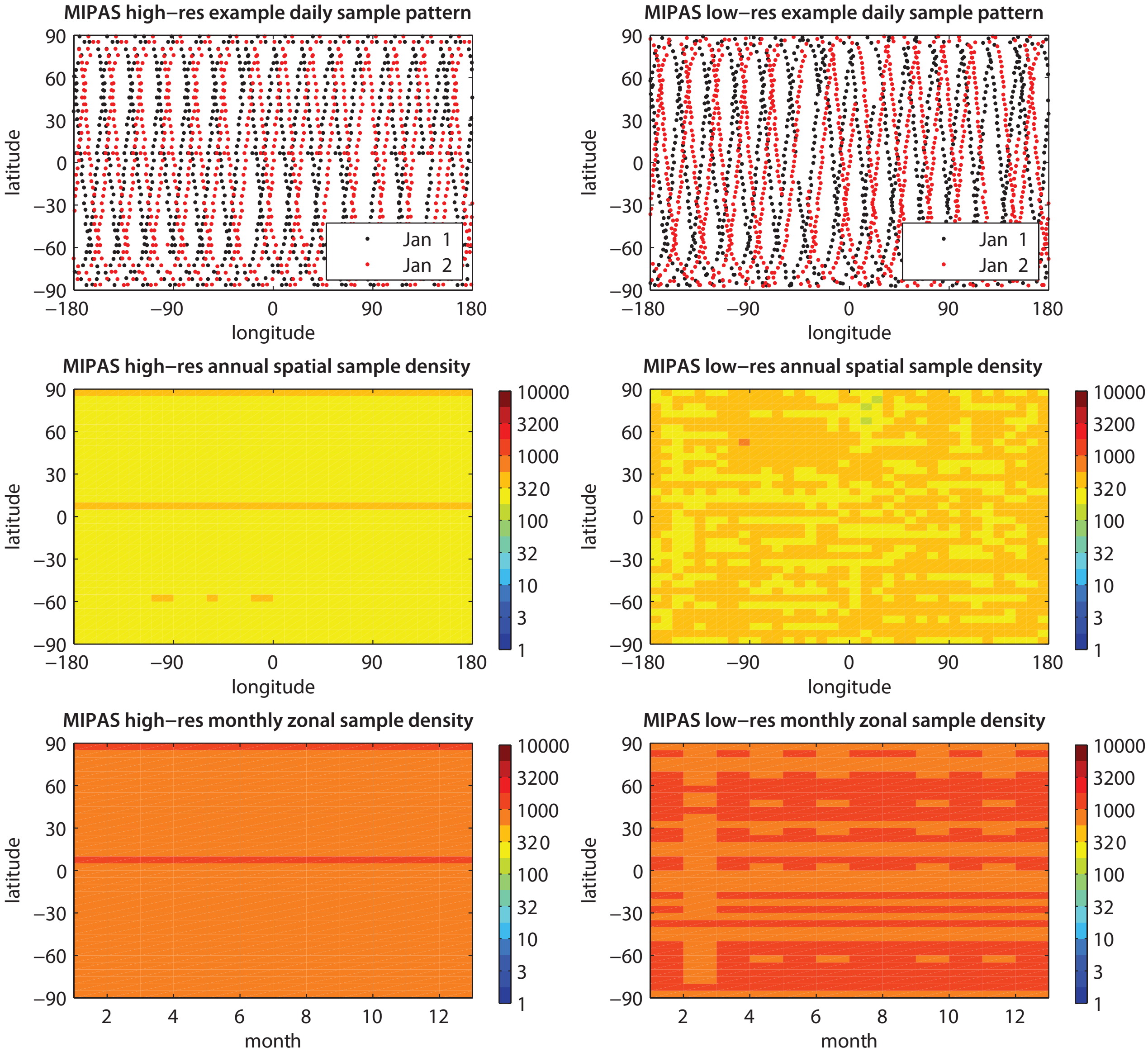

Figure 2.11: Sampling pattern and resulting sample density for MIPAS. *Left panels show results for the full (high)-spectral resolution mode from 2002-2004, right panels for the reduced (low)-spectral resolution mode from 2005-ongoing.*

altitudes at 70, 66, 62, 58, 54, 50, 46, 43, 40, 37, 34, 31, 29, 27, 25, 23, and then at 1.5 km steps from 21 to 6 km. Due to this modified measurement scenario the number of profiles increased by about 20%.

Trace gas profiles included in this climatology have been retrieved from calibrated geo-located limb emission spectra with the MIPAS Level 2 research processor developed and operated by the Institute of Meteorology and Climate Research (IMK) in Karlsruhe together with the Instituto de Astrofísica de Andalucía (IAA) in Granada. The general retrieval strategy, which is a constrained multi-parameter non-linear least squares fitting of measured and modelled spectra, is described in detail in *von Clarmann et al.* [2003c]. Its extension to retrievals under consideration of non-LTE (CO, NO, and NO_2) is described in *Funke et al.* [2001]. After wavenumber-recalibration, target quantities are retrieved sequentially, starting with temperature and LOS elevation (from CO_2 emissions around 15 µm), followed by the atmospheric main IR emitters H_2O, O_3, CH_4 and N_2O. Afterwards all other species are retrieved under consideration of the results of the preceding retrievals. Instead of the commonly used optimal estimation scheme, a Tikhonov-type first order regularisation is used [*Steck and von Clarmann*, 2001] because it does not constrain the column information but only how this information is distributed over altitude and, thus, does not push the mixing ratios towards *a priori* information. The strength of the regularisation is altitude dependent, with the aim of finding the best trade-off between the vertical resolution and the precision of the retrieved parameters. While trace gas abundances are retrieved in terms of VMR for most species, for some species (H_2O, NO_2, NO, CO), ln(VMR) is retrieved instead in order to better account for their pronounced temporal and spatial variability and reduce their dynamical range. Further, some target quantities (temperature and the trace gases NO, NO_2, and CO) are characterised by a pronounced spatial inhomogeneity, particularly close to transport barriers. In these cases, horizontal gradient profiles are taken into account within the retrieval [*Kiefer*, 2010]. In addition,

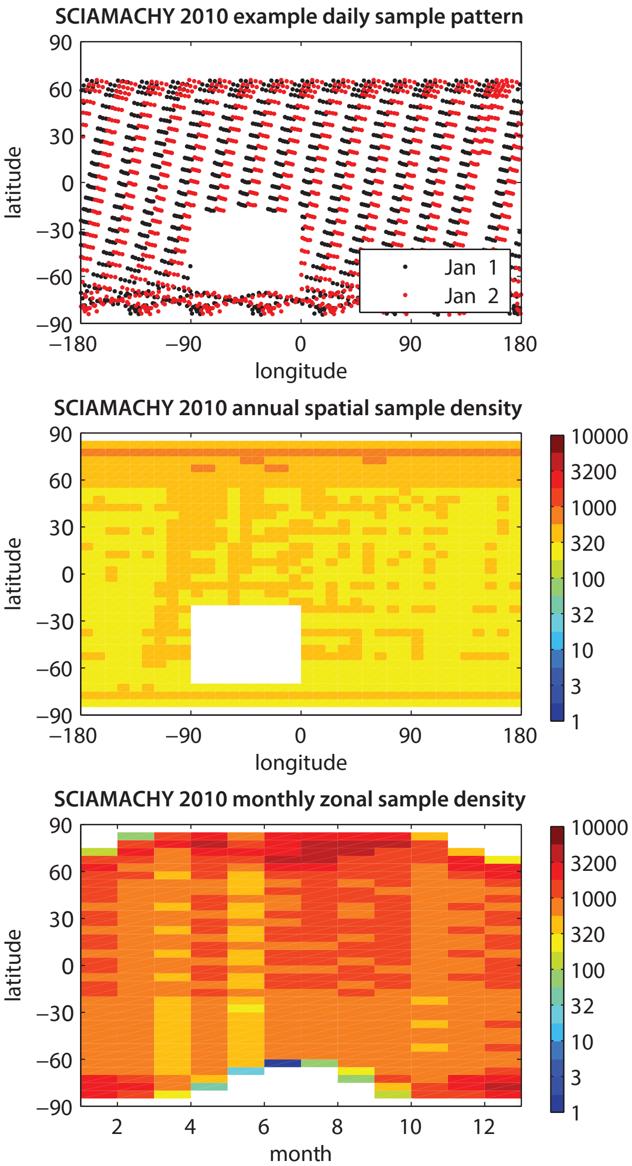

Figure 2.12: Sampling pattern and resulting sample density for SCIAMACHY.

a radiance offset and a continuum-like optical depth profile are fitted jointly for each microwindow in order to compensate for calibration errors and atmospheric contributions of weak wavenumber dependence not reproduced by the radiative transfer forward model [*von Clarmann et al.*, 2003c]. The MIPAS-IMK/IAA research data product, along with related diagnostics, is available to registered users *via* **http://www.imk-asf.kit.edu/english/308.php**. The sampling patterns and resulting measurement densities from MIPAS high and reduced spectral resolution measurement modes can be seen in **Figure 2.11**.

2.2.10 SCIAMACHY on Envisat

The Scanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) [*Burrows at al.*, 1995, *Bovensmann et al.*, 1999] was a payload on Envisat launched in March 2002 (for launch and orbit details, see *Section 2.2.8*). SCIAMACHY was one of the new-generation of space-borne instruments capable of performing spectrally-resolved measurements in several different modes: alternate nadir and limb observations of the solar radiation scattered by the atmosphere or reflected by the Earth's surface; and observations of the light transmitted through the atmosphere during solar or lunar occultation when feasible. The SCIAMACHY instrument was a passive imaging spectrometer comprised of eight spectral channels covering a wide spectral range from 214 to 2386 nm. Each spectral channel comprised a grating spectrometer, having a 1024-element diode array as a detector. Depending on the spectral channel the spectral sampling ranged from 0.11 to 0.74 nm and the spectral resolution from 0.22 to 1.48 nm.

This study uses SCIAMACHY measurements from scattered solar light in the limb-viewing geometry. In this geometry, the atmosphere was observed tangentially to the Earth's surface starting at about 4.5 km below the horizon (~1.5 km below the horizon since January 2011), *i.e.*, when the Earth's surface was still within the field-of-view of the instrument, and then scanning vertically up to the top of the neutral atmosphere (about 100 km tangent height). At each tangent height a horizontal scan of 1.5 s duration was performed followed by an elevation step of about 3.3 km. No measurements were performed during the vertical step. This results in a vertical sampling of 3.3 km. The vertical instantaneous field-of-view of the SCIAMACHY instrument was about 2.6 km at the tangent point. Although the horizontal instantaneous field-of-view of the instrument was about 110 km at the tangent point, the horizontal resolution was mainly determined by the integration time during the horizontal scan, reaching typically about 240 km. The entire distance at the tangent point covered by the horizontal scan was about 960 km. The along-track horizontal resolution was estimated to be about 400 km. In the nominal mode, about 100 measurements per orbit with 14 complete orbits per day were performed. Global coverage was achieved after six days. The sampling pattern and resulting data density for SCIAMACHY limb observations can be seen in **Figure 2.12**. The sampling pattern shown in **Figure 2.12** refers to standard retrievals with measurements at SZAs of up to 89°, resulting in a maximum latitude coverage of 65° in the winter hemisphere. This applies to all SCIAMACHY climatologies used in this study except for water vapour, for which only measurements at SZAs smaller than 85° are processed, resulting in a reduced latitude coverage of 55°. The gap in the sampling seen in the Southern Hemisphere is due to the South Atlantic anomaly. In this area the instrument electronics were exposed to an increased flux of energetic particles, which disturbed the measured signal resulting in a significant retrieval bias. This makes it necessary to reject the affected data when creating the climatologies (see *Section 3.1.3.10* for details).

Similar to other limb scattering instruments, the pointing uncertainty is a major error source. Currently, the accuracy of the pointing for the whole limb scan is estimated to be about 200 m. The relative pointing error between different tangent heights is negligible. The measurements at the lower tangent heights are affected by clouds; no retrievals can be done in the presence of a cloud in the instrument field-of-view.

More general information on the SCIAMACHY instrument can be found at **http://envisat.esa.int/instruments/sciamachy/** and **http://www.iup.physik.uni-bremen.de/sciamachy/**.

Vertical profiles of atmospheric species and aerosol extinction coefficients included in this climatology are retrieved from SCIAMACHY limb measurements using the scientific processor developed and operated by the Institute of the Environmental Physics (IUP) at the University of Bremen. Depending on the species, several spectral sub-windows in UV, visible, or near-infrared spectral ranges are used. Retrievals of O_3 and aerosol extinction coefficients exploit radiance profiles averaged over several nanometer wide spectral windows, whereas NO_2, BrO, and H_2O algorithms gain information from the differential structure of the trace gas absorption bands (DOAS technique). All retrievals except for H_2O use the reference tangent height normalisation technique to reduce the influence of the solar Fraunhofer lines, instrument calibration errors, and radiation scattered in the lower troposphere or reflected from the underlying surface. The retrieval relies on the optimal estimation type technique including an additional smoothing constraint (first order Tikhonov term). The non-linearity of the inverse problem is accounted for by employing the Gauss-Newton iterative scheme.

For most species, the retrieval is done for number densities while for H_2O the logarithms of the number densities are retrieved. Details on the retrieval algorithms and validation results for different species can be found in *Rozanov et al.* [2005], *Ernst et al.* [2009], *Sonkaev et al.* [2009], *Bauer et al.* [2012], *Mieruch et al.* [2012], *Rozanov et al.* [2011a; 2011b]. The SCIAMACHY scientific products retrieved by IUP Bremen are available to registered users *via* **http://www.iup.physik.uni-bremen.de/scia-arc**. Except for the aerosol extinction coefficients, the results are provided along with the averaging kernels, retrieval precision, and cloud flags.

2.2.11 ACE-FTS on SCISAT-1

The Atmospheric Chemistry Experiment-Fourier Transform Spectrometer (ACE-FTS), on board the SCISAT-1 satellite, uses mid-infrared solar occultation to investigate the chemical composition of the atmosphere [*Bernath*, 2006]. The SCISAT-1 satellite was launched on 12 August 2003 and routine measurements began on 21 February 2004. The ACE-FTS instrument is a high-resolution (0.02 cm^{-1}) FTS measuring the full spectral range between 13.3 and 2.2 μm (750 and 4400 cm^{-1}) [*Bernath et al.*, 2005]. The ACE-FTS measures approximately 15 sunrise and 15 sunset occultations per day and achieves global latitude coverage over a period of three months (*e.g.*, one "season"). The sampling pattern and resulting measurement density from the ACE-FTS can be seen in **Figure 2.13**. These spectral measurements extend from the cloud tops to 150 km. The vertical spacing between each 2-second ACE-FTS measurement varies between 1.5 and 6 km depending on the satellite's orbit geometry. The FOV of the instrument is approximately 3 km at the limb. Because of the high inclination of the SCISAT-1 orbit (74°), almost 50% of the occultation measurements made by the ACE-FTS are at latitudes of 60° and higher. The SCISAT-1 orbit was tuned to obtain a pattern of measurement latitudes that repeats each year. Thus, as noted below, the sampling pattern and density of measurements are representative for all years of the SCISAT-1 mission.

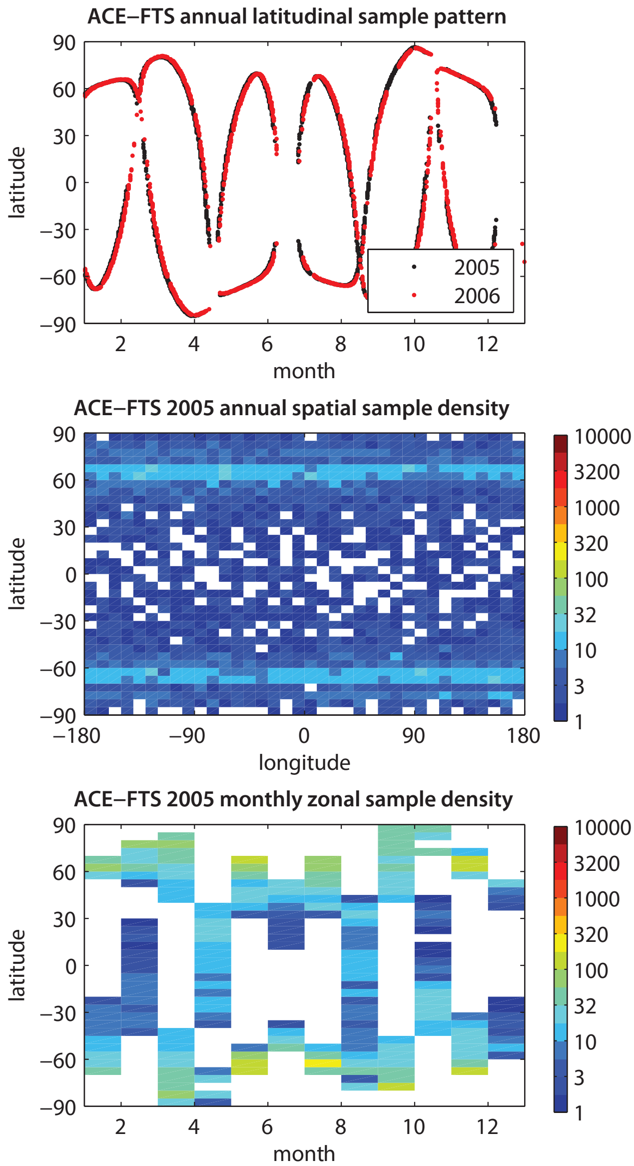

Figure 2.13: Sampling pattern and resulting sample density for the ACE-FTS. *The sampling corresponds to the year 2005, which is representative for all years.*

Exo-atmospheric and deep space spectra recorded during each occultation are used to calculate atmospheric transmission spectra from the ACE-FTS measurements. The use of transmission spectra provides "self-calibration" for these occultation measurements. It makes the ACE-FTS dataset less susceptible to changes over the mission and provides very good long-term stability in the measurements.

Level 2 constituent profiles are retrieved from the ACE-FTS transmission spectra in VMR using an unconstrained non-linear least squares global fitting approach [*Boone et al.*, 2005, and references therein]. In the first step, CO_2 lines in the spectra are used to determine the pressure and temperature as a function of altitude. The micro-windows used for the retrieval cover the following wavenumber ranges: 932–937, 1890–1976, 2042–2073, 2277–2393, 2408–2448, 3301–3380, and 3570–3740 cm^{-1}. Temperature and pressure profiles are retrieved from the ACE-FTS spectra between 12 and 120 km. Below 12 km, meteorological results from the Canadian Meteorological Centre operational weather analysis and forecast system are used. Above 120 km, output from the Naval Research Laboratories MSISE-00 software is employed. The resulting temperature and pressure profiles are used to retrieve VMR profiles of over 30 trace gas species from sets of micro-windows chosen to contain spectral features specific to each of the target molecules. The spectroscopic parameters used for these calculations are from the HITRAN 2004 linelist [*Rothman et al.*, 2005]. The retrieval algorithm uses first guess profiles taken from the four ATMOS missions on-board the Space Shuttle. However, the retrievals are not constrained by these first guess profiles. Currently, there is no error budget available for the ACE-FTS products. For each measurement, there is an associated fitting uncertainty provided. This one-sigma fitting uncertainty is the square root of the diagonal element of the covariance matrix obtained in the retrieval process [*Boone et al.*, 2005]. A document describing the microwindows used for the ACE-FTS retrievals is available from **http://www.ace.uwaterloo.ca** [ACE Report ACE-SOC-0020, Microwindow List for ACE-FTS retrievals – Version 2.2 + updates, Dec. 2006].

For the SPARC Data Initiative, the ACE-FTS Version 2.2 data products are used including updates for O_3 and N_2O_5. The validation results for these species and parametres are included in a special issue of Atmos. Chem. Phys. (**http://www.atmos-chem-phys.org/special_issue114.html**). In addition, two climatologies have been created for the 2004-2009 period using the Version 2.2 (plus updates) dataset: a climatology for O_3, H_2O, CH_4, N_2O, CO, NO, NO_2, N_2O_5, HNO_3, HCl, $ClONO_2$, CCl_3F, CCl_2F_2, and HF [*Jones et al.*, 2012] and an NO_y climatology derived from the ACE-FTS NO, NO_2, HNO_3, HNO_4, N_2O_5 and $ClONO_2$ products [*Jones et al.*, 2011]. Both are five-year zonal mean climatologies provided on a monthly and three-month basis. The Level 2 ACE-FTS data products are stored by occultation in ASCII format (main isotopologues and minor isotopologues are in separate files for each occultation). Further information about ACE-FTS and the ACE mission, including the Level 2 Version 2.2 data products, can be found at: **http://www.ace.uwaterloo.ca/**.

2.2.12 ACE-MAESTRO on SCISAT-1

The Measurement of Aerosol Extinction in the Stratosphere and Troposphere Retrieved by Occultation (MAESTRO) is a dual UV/VIS/Near-IR spectrophotometer that is part of the Atmospheric Chemistry Experiment (ACE) mission on-board the SCISAT-1 satellite [*McElroy et al.*, 2007]. ACE-MAESTRO was designed to extend the ACE wavelength coverage to the 280-1030 nm spectral region using two spectrometers with overlapping coverage (280-550 nm, 500-1030 nm) to reduce stray light. Currently, it makes measurements of solar radiation between 450-1030 nm during each sunrise and sunset with a spectral resolution of 1-2 nm (depending on spectral region). The two ACE instruments take simultaneous measurements of the same air mass using a common sun-tracking mirror that is located within the ACE-FTS. During each occultation (sunrise or sunset measurement), approximately 60 spectra are measured by ACE-MAESTRO between the cloud tops and 100 km. The vertical spacing of these measurements varies from 300 m to 2 km at altitudes below 50 km and the spacing increases to every 5 km for altitudes above 50 km. The FOV of the instrument is approximately 1 km at the limb.

As noted in *Section 2.2.11*, the SCISAT-1 satellite was launched on 12 August 2003 and began routine measurements on 21 February 2004. The sampling pattern and resulting measurement density from ACE-MAESTRO is essentially identical to that of ACE-FTS (as shown in **Figure 2.13**). As can be seen in **Figure 2.13**, ACE-MAESTRO achieves global latitude coverage in its measurements over a period of three months.

Level 2 profiles of O_3, NO_2, and optical depth are retrieved from the ACE-MAESTRO measurements as a function of altitude using a differential optical method combined with an interactive Chahine relaxation inversion algorithm [*McElroy et al.*, 2007, and references therein]. In the first step, the raw data are converted to wavelength-calibrated spectra, corrected for stray light, dark current and other instrument parameters. Then, a non-linear least-squares spectral fitting routine is used to analyse the corrected spectra. These are used to calculate slant-path column densities for each spectrum and, from these, vertical profiles of O_3 and NO_2 VMRs are derived by adjusting an initial guess profile from a high-vertical-resolution model simulation. Pressure and temperature profiles used in the ACE-MAESTRO retrievals are obtained from the corresponding ACE-FTS occultation measurement and are used to fix the tangent heights for the ACE-MAESTRO retrievals. The retrieval algorithm does not require any *a priori* information or other constraints [*McElroy et al.*, 2007]. No error budget has been produced for the ACE-MAESTRO data products. For each measurement, there is an associated error provided. This is essentially the random error of the measurement and is produced by propagating the instrument noise through the spectral fitting and profile retrieval codes.

For this project, the ACE-MAESTRO Version 1.2 O_3 data products are used, which are available from: **http://www.ace.uwaterloo.ca**. The Level 2 ACE-MAESTRO data products for each species/parameter are stored individually by occultation in ASCII format. The validation of the ACE-MAESTRO ozone product was described by *Dupuy et al.* [2009] and is part of the special issue of Atmospheric

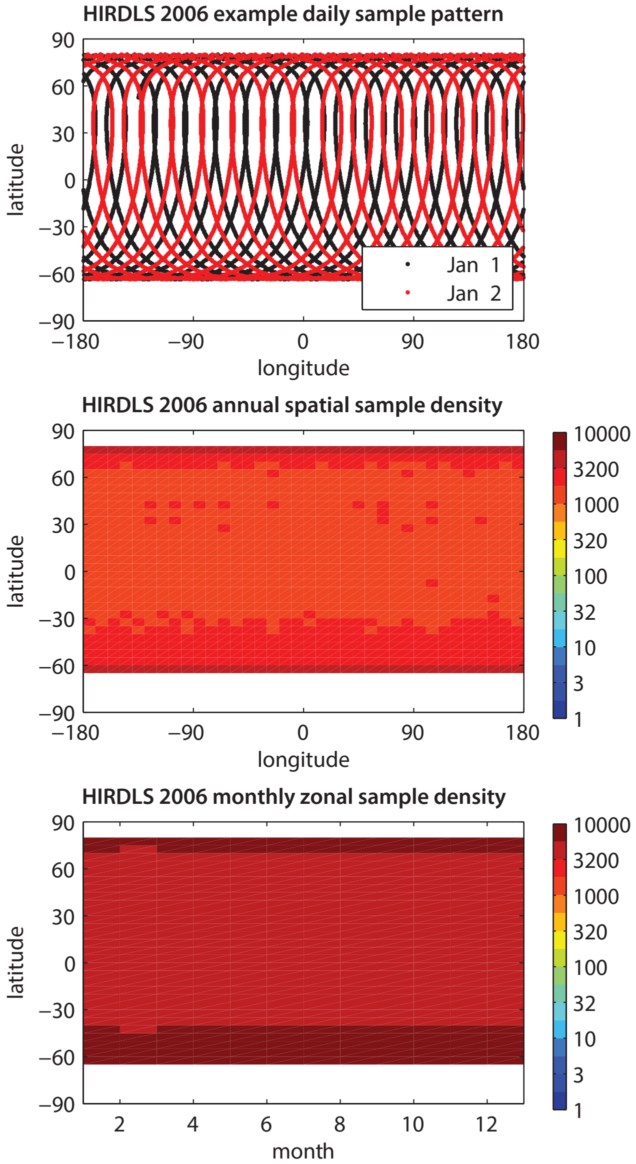

Figure 2.14: Sampling pattern and resulting sample density for HIRDLS.

Chemistry and Physics (described above: **http://www.atmos-chem-phys.org/special_issue114.html**).

2.2.13 HIRDLS on Aura

The High Resolution Dynamics Limb Sounder (HIRDLS) instrument is a 21-channel limb-scanning infrared radiometer, designed to scan from the upper troposphere into the mesosphere and provide data with 1-km vertical resolution. HIRDLS was launched on the Aura satellite into a polar orbit on July 15, 2004 (see *Section 2.2.15*). The original description of the experiment is by *Gille and Barnett* [1992]. Its channels cover the wavelength range from 6.12 to 17.76 µm, or 563 -1634 cm^{-1}, in order to measure emission features from 11 trace gases and from aerosols. Four channels measure emission by CO_2, from which temperature is recovered as a function of pressure. Three channels are dedicated to the retrieval of O_3, two to H_2O, and one each to CH_4, N_2O, NO_2, N_2O_5, HNO_3, $ClONO_2$, CFC-11 and CFC-12, with others for measurement of aerosols at four wavelengths. The large number of channels allows several to be dedicated to obtaining measurements in weaker parts of the bands, allowing sounding of the upper troposphere.

Unfortunately, HIRDLS was damaged during launch such that most of the aperture was covered. The blocking material is believed to be a thin film of plastic that became dislodged during launch and settled in the optical train, blocking 80-95% of the beams leading to the 21 detectors. In addition to blocking the aperture areas, this material gives off radiance signals that vary with scan angle and time on many scales. *Gille et al.* [2008] give a post-launch description of HIRDLS. Data coverage is from 63°S to 80°N, with profiles spaced every 100 km along the scan track, as shown in **Figure 2.14**. Because three of the retrieved species have diurnal variations, it is also important to know the local time of the retrievals on the ascending (northward) and descending portions of the orbit. *Gille et al.* [2008] also describes the initial corrections that resulted in Version 3 (V3) data. While details have changed, the procedure is the same for the V6 data discussed here.

Vertical coverage varies for each species, but the 1 km vertical resolution has been preserved. Persistent effort has resulted in successive improvements, leading to the release of the V6 data relevant to this report. They include temperature, O_3, HNO_3, CFC-11, CFC-12, and zonal means of day (1500 UT) and night (0 UT) NO_2, and night N_2O_5. All products for a single day are in a single file, on a grid of 24 pressure levels per decade of pressure, uniformly distributed in log pressure. More detailed characteristics of these data are included in the Data Description and Quality Document, Version 6, available from **http://archive-eos.acom.ucar.edu/hirdls/**, **http://disc.sci.gsfc.nasa.gov/data-holdings**, or **http://badc.nerc.ac.uk/browse/badc/hirdls**.

HIRDLS data are calibrated, corrected and retrieved in two major processors. In the first, the L1 processor, the conversion from raw counts to corrected radiances takes place, and the scans are geo-located. Subsequently they are corrected for the effects of the blocking material. The first correction is the removal of the small amplitude oscillations at ~1.8 Hz, which are initiated when the scan mirror contacts the plastic film during a scan. Next, the signal emitted by the film is removed, based on measurements made when Aura is pitched so that the complete HIRDLS scan is above the atmosphere, and only the film is viewed. Finally, the signal is corrected for the reduced effective aperture. Recent efforts have been made to model more closely the signal from the film, especially its change over the 3-year mission. After these corrections are made, the input radiances are on a nearly unifom elevation angle scale with a spacing that corresponds to ~200 m at the limb. They are then filtered to remove noise at spatial frequencies too high to be seen by HIRDLS, then splined onto an altitude grid with 1 km spacing. Channel 6 near 830 cm^{-1} is in the most transparent portion of the spectrum; it is used for the detection of clouds and aerosols. The altitude at which channel 6 radiances

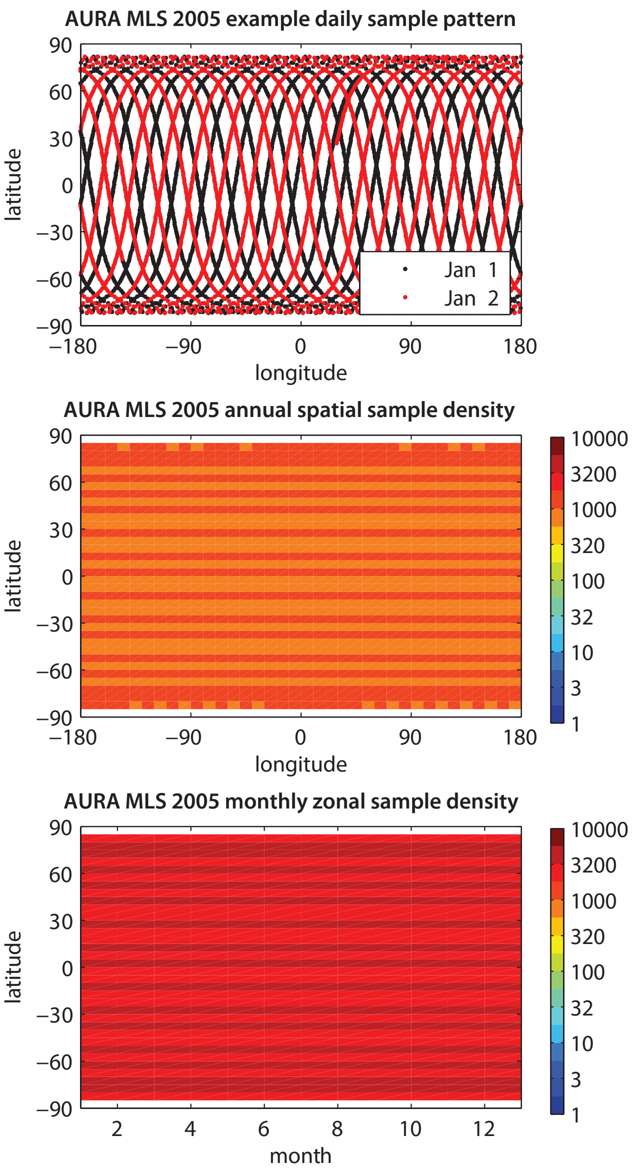

Figure 2.15: Sampling pattern and resulting sample density for Aura-MLS.

suddenly increase is tagged as the cloud top, but it is verified and possibly adjusted with data from channel 12. These are input to the second step, the L2 retrieval processor.

The retrieval algorithm is based on optimal estimation theory [*Rodgers*, 2000], using a modified Levenberg-Marquardt approach for the iterative solution. The application for HIRDLS is described in detail in *Khosravi et al.* [2009]. The L2 step accepts the conditioned radiance data from the L2CLD, where cloud top heights are determined, and performs the retrievals through a series of iterations. This code is designed to be flexible in handling combinations of radiance channels to retrieve the HIRDLS target species in a user-defined sequence. One of the major features is the use of ancillary data from the Goddard Earth Observing System Model (GEOS-5), produced by NASA's Global Modeling and Assimilation Office (GMAO) to determine temperature gradients along the LOS, which are incorporated to yield improved retrievals. This processor is described in detail in the L1-2 Algorithm Theoretical Basis Document (ATBD) available on the web at **http://archive-eos.acom.ucar.edu/hirdls/data/products/HIRDLS-DQD_V6-1.pdf**. GEOS-5 Version 5.01 data were used through January 2, 2008, after which Version 5.1 data were used.

2.2.14 MLS on Aura

Aura-MLS is a Microwave Limb Sounder (MLS) instrument, which is part of the Earth Observing System (EOS) and launched on the Aura satellite on 15 July 2004 (for orbit details, see *Section 2.2.15*). Aura-MLS, like its predecessor version on the UARS (see *Section 2.2.4*), measures microwave thermal emission day and night, simultaneously from several spectral regions, using an antenna that scans the Earth's atmospheric limb, in this case every 24.7 s.

Aura-MLS measures thermal emission from the limb in five broad spectral regions between 118 GHz and 2.5 THz. Aura-MLS views the atmosphere ahead of the Aura satellite, which is in a sun-synchronous near-polar orbit, with a ~1:45pm equatorial crossing time (ascending node). The MLS vertical scans are synchronised to the Aura orbit, leading to retrieved profiles at the same latitude every orbit, with a spacing of 1.5° great circle angle (about 165 km) along the sub-orbital track; the horizontal (along-track) resolution is limited by the smearing of sensitivity near the tangent point, including the impact of retrieval smoothing constraints, but typically ranges from 200 to 500 km in the stratosphere. The 240 limb scans per orbit provide almost 3500 profiles (per species) every day, from about 82°S to 82°N. The sampling pattern and resulting measurement density from Aura-MLS can be seen in **Figure 2.15**. The vertical retrievals are typically on a pressure grid with six levels (pressure surfaces) per decade change in pressure in the stratosphere and lower mesosphere; the main Version 3.3 exception relevant for (and used in) this report is the H_2O product, which is retrieved on a vertical grid that is twice as fine as that for most other species.

The Aura-MLS retrievals use the "optimal estimation" method [*Rodgers*, 1976; 2000]. This involves the nonlinear weighted least squares optimisation of a cost function describing the fit to observed radiance signals, including the use of *a priori* constraints for regularisation. Uncertainty estimates are provided as a result of the inversion process, based on input radiance uncertainties and *a priori* profile uncertainties. Gauss-Newton iteration is used, with a second order Tikhonov constraint [*Tikhonov*, 1963]; this constraint is applied to the profile second derivatives (vertically and horizontally). Specific retrieval aspects include adaptation to a two-dimensional system, using the LOS measurements from several scans to derive information about several profiles [see *Livesey and Read*, 2000]. The various species are retrieved from overlapping "chunks" of observations, typically consisting of a 15° span of great circle angle (about ten vertical scans). Several retrieval "phases" are performed in sequence, each using a different set of measured radiances; some phases retrieve temperature and pressure, and some include this information from an earlier phase. In the MLS retrieval system, the state vector represents vertical profiles of mixing ratios in a piecewise-linear manner. The only exception is water vapour, where the representation is piecewise-linear in the logarithm of the VMR, nevertheless the retrieved quantity is VMR.

The Aura-MLS Level 2 data files include various screening flags to provide users with information about instrument and retrieval status (and also about quality of fit and retrieval convergence) based on various criteria described in the species-specific V2.2 validation papers. The updated V3.3 retrievals used to generate the SPARC Data Initiative climatologies for this report (except for ozone, for which V2.2 is recommended overall because of vertical oscillations that exist primarily in V3.3 in the UTLS at low latitudes) follow generally the same (V2.2) flagging/screening methodologies and recommendations for data usage, albeit with some changes in the screening flag threshold values. Also, the V3.3 data for CO and HNO_3 (used here) are more sensitive to cloud effects than previous versions, as a result of changes in the retrieval approach and the vertical range used in the UT. The resulting data screening methods include the removal of negative outliers (spikes of a certain size), as described in the V3.3 Aura MLS Data Quality documentation [*Livesey et al.*, 2011]. The impact of clouds depends on cloud thickness and altitude, and this mostly affects the species retrieved at low latitudes in the UTLS. The fraction of (daily) discarded profile values in these regions is typically 5 to 10%, and occasionally more than 20%. Different sensitivities to clouds can, in effect, lead to sampling biases between instruments; other satellite sensors are typically more affected by clouds and humidity than those in the microwave region. More details about the Aura-MLS retrieval approach are provided by *Livesey et al.* [2006] and calculation specifics of the Aura-MLS radiance model ('forward model') are described by *Read et al.* [2006] and *Schwartz et al.* [2006]. *Waters et al.* [2006] provide a detailed description of the Aura-MLS instrument's characteristics, spectral bands, and geophysical profile measurements.

Level 2 daily profiles are stored in Level 2 data files (one file per parameter) in Hierarchical Data Format (HDF-EOS 5 format type), and available from the NASA Goddard Spaceflight Center Distributed Active Archive Center (DAAC), specifically the Goddard Earth Sciences (GES) Data and Information Services Center (DISC), at the Mirador website, namely **http://mirador.gsfc.nasa.gov**. Information about MLS, data access, and MLS-related publications, can be found at the MLS website (**http://mls.jpl.nasa.gov**). The Aura-MLS data quality documentation [*Livesey et al.*, 2011] is available at **http://mls.jpl.nasa.gov/data/v3-3_data_quality_document.pdf**.

2.2.15 TES on Aura

The Tropospheric Emission Spectrometer (TES) is a Fourier Transform Spectrometer that was launched on the NASA Earth Observing System (EOS) Aura satellite in 2004 [*Beer*, 2006; *Beer et al.*, 2001]. The Aura satellite has a 705 km sun-synchronous polar orbit with an inclination of 98.21°, which provides global coverage from 82°S to 82°N with equator crossing times of 1:43pm (ascending node) and 1:43am (descending node) and a 16 day repeat cycle. TES measures spectrally-resolved thermal infrared radiation (650-3050 cm^{-1}) with a spectral resolution of 0.06 cm^{-1} (unapodised) in the nadir mode. TES covers this spectral range with four filters: 2B1 (650-900 cm^{-1}), 1B2 (950-1150 cm^{-1}), 2A1 (1100-1325 cm^{-1}), and 1A1 (1900-2250 cm^{-1}), and measures surface and atmospheric temperature as well as a variety of trace gases including O_3, CO, H_2O, HDO, CH_4, CO_2, NH_3, CH_3OH, and HCOOH, with greatest sensitivity in the troposphere. TES supports both nadir and limb scanning modes, but the limb measurements were discontinued in May 2005 in order to extend the life of the instrument. TES observes multiple spectra through a linear array of 16 pixels. At the nadir, the spatial resolution of each pixel is 0.5 x 5 km and is averaged to a footprint of 5.3 x 8.5 km, with a separation of ~182 km. TES is a pointable instrument and can access any target within 45° of the local vertical,

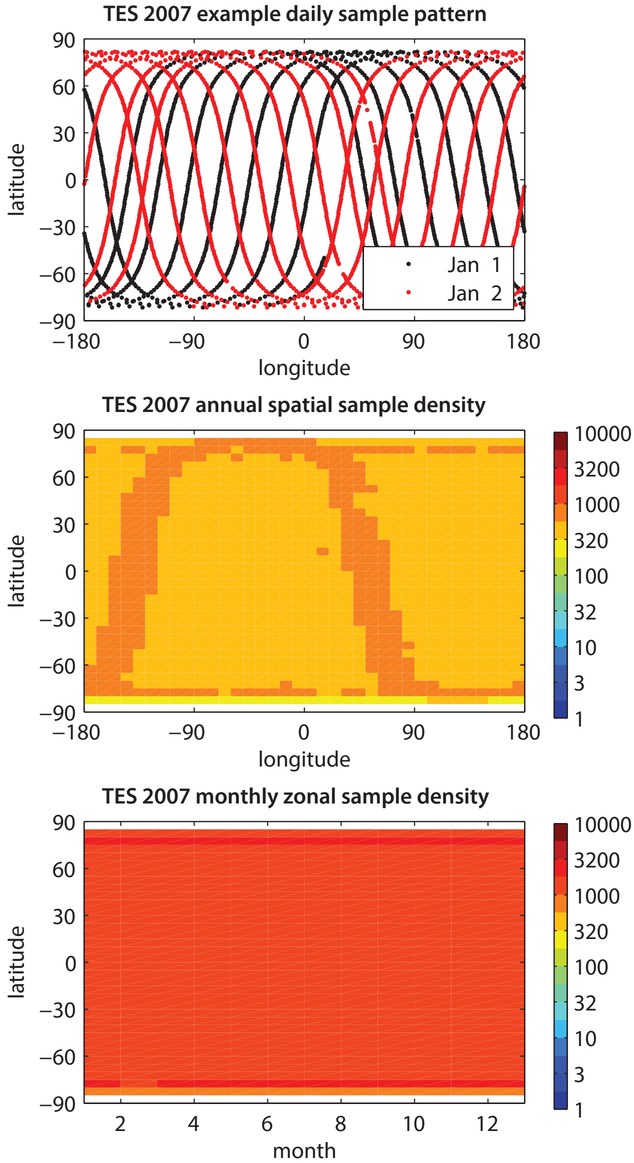

***Figure 2.16:** Sampling pattern and resulting sample density for TES before June 2008.*

allowing for more tightly spaced measurements during Special Observations modes. Here we use only the standard nadir-viewing Global Survey O_3 measurements, with near-global coverage in 16 orbits (~26 hours) (see **Figure 2.16**). In cloud-free conditions, TES nadir O_3 profiles have approximately 4 degrees of freedom for signal, with ~2 in the troposphere and ~2 in the stratosphere (below ~5 hPa). This is equivalent to a vertical resolution of ~6-7 km.

TES sampling has changed over the mission lifetime in response to instrument aging. To extend the life of the instrument, the latitudinal coverage was reduced in June 2008 to 60°S-82°N and in July 2008, to 50°S-70°N. From January to April 2010, the instrument went offline due to problems with the scanning mechanism. When operations resumed in May 2010, the latitude coverage was further reduced to 30°S-50°N and the calibration strategy was changed from multiple black body scans per orbit to two sets of black body scans per day to reduce wear on the pointing mechanism of the instrument. This reduction in the number of calibration scans resulted in a 25% increase in the number of observations per global survey and regular but non-uniform spacing between the measurements (ground track separation cycles through 56 km, 195 km, 187 km, and 122 km and then returns to 56 km). A second data gap of approximately three weeks occurred in October 2010, with only two Global Surveys conducted that month. Since April 2011, data gaps became more common as the instrument continues to age.

TES retrievals and error estimation are described in *Worden et al.* [2004], *Bowman et al.* [2002, 2006], and *Kulawik et al.* [2006a]. The optimal estimation retrieval method that is used [*Rodgers*, 2000] is based on minimising the difference between observed radiances and a radiative transfer model subject to *a priori* constraints. Use of optimal estimation provides detailed characterisation of the smoothing, random, and systematic errors for the target parameters as well as important retrieval metrics such as degrees of freedom, information content, and vertical resolution. The radiative transfer model is referenced with respect to the logarithm of pressure (67 levels with a geometric layer thickness of 0.6-0.8 km from 100-1 hPa and 1.5 km above 1 hPa), with surface temperature, emissivity, and clouds included in the forward model. Spectral windows are selected to reduce the computational load and minimise systematic errors from non-retrieved atmospheric parameters. The TES retrieval strategy begins with updates to surface temperature and cloud parameters based on brightness temperature in a window region near 10 μm. Ozone is jointly retrieved with water vapour (both in ln(VMR) to account for their large dynamic range) following CO_2 and temperature on a subset of the 67-level forward model pressure grid. Each retrieval step includes the constituent of interest, interferents, and cloud and surface parameters, and the subset of vertical levels is chosen so as to capture the expected vertical variations of the retrieved trace gas. *A priori* profiles for temperature and water vapour are taken from the GEOS global circulation model of NASA's Global Modeling and Assimilation Office (GMAO), and initial profiles for O_3 are taken from the MOZART Chemistry-Transport Model [*Brasseur et al.*, 1998, *Park et al.*, 2004]. Constraint matrices are based on the altitude-dependent Tikhonov constraint and covariances from MOZART [*Kulawik et al.*, 2006b]. The least squares minimisation is based on the trust-region Levenberg-Marquardt algorithm [*Moré*, 1977] and subject to the constraint that the estimated state must be consistent with *a priori* probability distribution for that state. TES data, including averaging kernels and error covariance matrices, are publicly available. For more information, see **http://tes.jpl.nasa.gov/**.

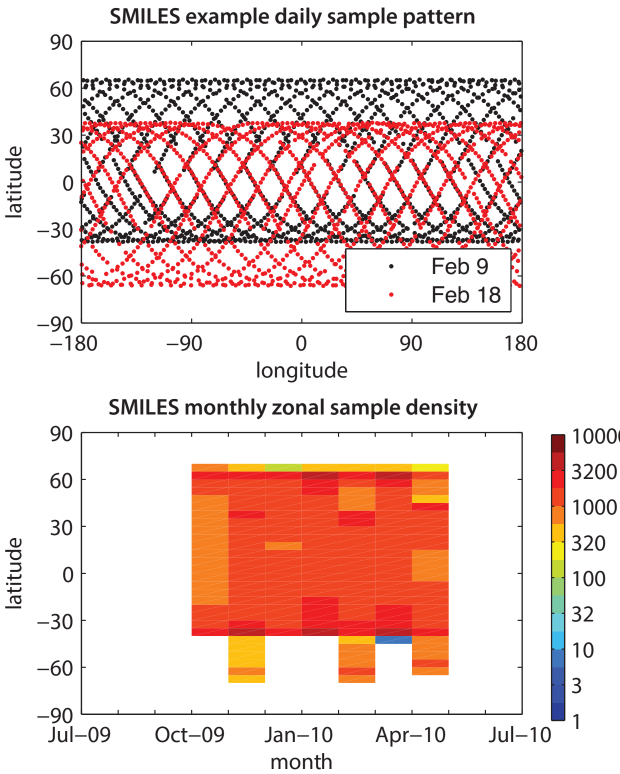

Figure 2.17: Sampling pattern and resulting sample density for SMILES.

2.2.16 SMILES on the ISS

SMILES (Superconducting Submillimeter-Wave Limb Emission Sounder) was selected as a first Earth observation mission for the Exposed Facility (EF) of the Japanese Experiment Module (JEM) on the International Space Station (ISS) in 1997, where it was installed on 25 September 2009. The purpose of the SMILES instrument was the demonstration of the ultra sensitive sub-mm limb emission observation with a 4-K cooled receiver system [*Kikuchi et al.*, 2010]. SMILES targeted atmospheric constituent observations such as for O_3, O_3 isotopomers, O_3 in the vibrational excited state, $H^{35}Cl$, $H^{37}Cl$, ClO, HNO_3, CH_3CN, HOCl, HO_2, and BrO in the stratosphere and mesosphere. Water vapour and ice clouds were observed in the UTLS. H_2O_2 and HOBr were also observed in the stratosphere and mesosphere although their spectrum signals are weak. The non-sun-synchronous orbit of the ISS allowed the instrument to observe the diurnal variation of these minor species. Observations

Table 2.3: Data versions of SMILES research products.

Data	Version	Availability	Comments
L1b	006	Feb 2011	Improved: AOS response function Problem: Calibration non-linearly
	007	June 2011	Improved: Calibration non-linearly Problem: Tangent height and latitude/longitude
L2r	201	Nov 2011	L1b data: Version 006 Altitude region: 24-90 km Problem: Spectrum calibration non-linearly
	215	Oct 2011	L1b data: Version 007 Altitude region: 12-90 km Improved: Spectrum calibration non-linearly Problem: Tangent height and latitude/longitude

were made by SMILES between 12 October 2009 and 21 April 2010, when SMILES stopped operations due to the failure of the local oscillator and the 4-K cooler. SMILES is a cooperative mission of the Japan Aerospace Exploration Agency (JAXA) and the National Institute of Information and Communications Technology (NICT). Details of the mission are described in the SMILES Mission Plan, Version 2.1, (**http://smiles.nict.go.jp/Mission_Plan/**).

The platform (ISS) altitudes are typically between 350 and 400 km. The altitude region of the antenna scan is from -10 to 120 km (nominal). The scanning altitude region of the observation was changed due to the change of the altitude, rotation, and vibration of the ISS platform. The antenna FOV is 0.009° (about 3-4 km). The SMILES instrument employs two superconductor-insulator-superconductor (SIS) mixers cooled at about 4 K and high-electron-mobility-transistor (HEMT) amplifiers at 20 and 100 K, cooled by a mechanical cryo-cooler. SMILES has two spectrometers. There are three observation frequency regions, band A: 624.32-625.52 GHz, band B: 625.12-626.32 GHz, and band C: 649.12-650.32 GHz. The transition of O_3 at 625.37 GHz was observed in both bands A and B for comparison/validation purposes. $H^{35}Cl$ was observed in band B, and $H^{37}Cl$ was observed in band A. Details of the frequency allocation are described in the SMILES Mission Plan, Version 2.1 (**http://smiles.nict.go.jp/Mission_Plan/**).

Since the ISS orbit is circular, with an inclination of 51.6°, the highest latitude reached by the ISS orbit is 52°N and S. To extend the latitudinal coverage to the northern higher latitudes, the SMILES antenna is mounted so that its FOV is 45° to the left of the orbital plane. The observed latitude region was between 38°S and 65°N (nominal). 1630 observation points were obtained per day, resulting in a sampling pattern as shown in **Figure 2.17**.

Trace gas profiles used for the SPARC Data Initiative climatologies have been retrieved from calibrated limb emission spectra with the SMILES Level 2 research processing system developed and operated by the National Institute of Information and Communications Technology (NICT). NICT developed an algorithm, named AMATERASU, to retrieve the vertical profiles of the atmospheric constituents from the calibrated limb emission spectra in the frequency region 624.32-625.52 GHz, 625.12-626.32 GHz, and 649.12-650.32 GHz. The maximum *a posteriori* (MAP) method with the Gauss-Newton interactive procedure modified by Levenberg has been adopted as the retrieval for O_3, HCl, ClO, HNO_3, CH_3CN, HOCl, HO_2, H_2O_2, BrO, and HOBr in the stratosphere and mesosphere, as well as H_2O and ice- cloud in the UTLS. Observations from the ISS generally suffer pointing problems. While the pointing information and temperature are commonly retrieved from molecular oxygen lines, there is no oxygen line in the SMILES spectral region. The retrievals of the LOS elevation angles and of temperature have been obtained from the strong ozone line at 625.371 GHz. For Version 2.1.5, it was pointed out by *Baron* [2011] that "The pointing parameters and the ozone profiles are retrieved from the line wings which are measured with high signal to noise ratio, whereas the temperature profile is retrieved from the optically thick line center. The main systematic component of the retrieval error was found to be the neglect of the non-linearity of the radiometric gain in the calibration procedure. This causes a temperature retrieval error of 5-10 K. Because of these large temperature errors, it is not possible to construct a reliable hydrostatic pressure profile. However, as a consequence of the retrieval of pointing parameters, pressure induced errors are significantly reduced if the retrieved trace gas profiles are represented on pressure levels instead of geometric altitude levels". The Level 2r Version 2.1.5 products for the SPARC Data Initiative suffer from the non-linearity problem of the radiometric gain in the calibration procedure of the spectrum. The error of the latitude-longitude position was estimated to be of the order of about 10-50 km.

The AMATERASU algorithm Version 2 series including V2.0.1 and V2.1.5 used only the clear-sky part of the radiative transfer calculation. The continuum component used the modified Pardo approach [*Pardo et al.*, 2001]. Although the continuum including H_2O is retrieved, the altitude region between about 16 and 90 km is maintained for the atmospheric composition. The "definitive window method" is used for the retrieval frequency range in order to obtain more accurate values in the stratosphere and mesosphere. The details of the retrieval method are described in *Baron et al.* [2011] for the Version 2 series of the SMILES research products, and the evaluation and validation status are discussed further in *Sato et al.* [2012] and *Kasai et al.* [2013].

The SMILES research data product is, along with related diagnostics, available to registered users *via* **https://data.smiles.nict.go.jp/products/research_latitude-longitude.jsf**.